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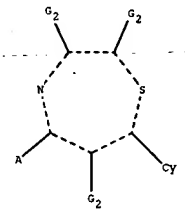

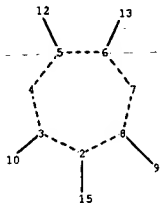

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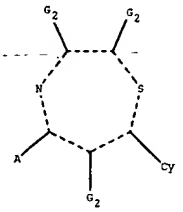
9
ring nodes :
2 3 4 5 6 7 8
ring/chain nodes :
10 12 13 15
chain bonds :
2-15 5-12 6-13 8-9
ring/chain bonds :
3-10
ring bonds :
2-3 2-8 3-4 4-5 5-6 6-7 7-8
exact/norm bonds :
2-3 2-8 2-15 3-4 3-10 4-5 5-6 5-12 6-7 6-13 7-8 8-9

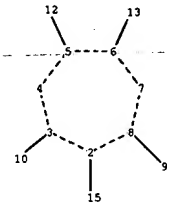
G1:O,S,N

G2:A,H

Match level :
2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:CLASS
12:CLASS 13:CLASS 15:CLASS

C:\STNEXP4\QUERIES\09836548.str





chain nodes :
9
ring nodes :
2 3 4 5 6 7 8
ring/chain nodes :
10 12 13 15
chain bonds :
2-15 8-9
ring/chain bonds :
3-10 5-12 6-13
ring bonds :
2-3 2-8 3-4 4-5 5-6 6-7 7-8
exact/norm bonds :
2-3 2-8 2-15 3-4 3-10 4-5 5-6 5-12 6-7 6-13 7-8 8-9

G1:O,S,N

G2:A,H

Match level :
2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:CLASS
12:CLASS 13:CLASS 15:CLASS

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=> d his

     (FILE 'HOME' ENTERED AT 12:57:35 ON 30 OCT 2002)

     FILE 'REGISTRY' ENTERED AT 12:57:43 ON 30 OCT 2002

     FILE 'STNGUIDE' ENTERED AT 13:01:01 ON 30 OCT 2002

     FILE 'REGISTRY' ENTERED AT 13:04:21 ON 30 OCT 2002
L1                STRUCTURE UPLOADED
L2                QUE L1
L3             21 S L2
L4           1885 S L2 SSS FUL
L5                STRUCTURE UPLOADED
L6                QUE L5
L7             11 S L6  SUB=L4 SAM
L8            185 S L6  SUB=L4 FUL
L9           1700 S L4 NOT L8
L10          9574 S C6-C5NS/EA
L11          1373 S L9 AND L10
L12           327 S L9 NOT L11

     FILE 'CAPLUS' ENTERED AT 13:11:37 ON 30 OCT 2002
L13            21 S L8
L14           426 S L11
L15            80 S L12
                  SAVE L14 A09836548/A
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=> d l2
L2 HAS NO ANSWERS
L1                STR
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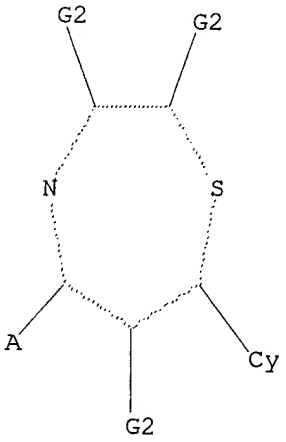
thiazepines

benzothiazepines

polycyclics

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G1 O,S,N
G2 A,H


Structure attributes must be viewed using STN Express query preparation.
L2                QUE  ABB=ON  PLU=ON  L1


=> d l5

Page 1
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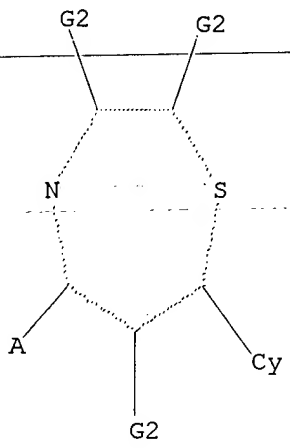
L5 HAS NO ANSWERS
L5 STR



G1 O,S,N
G2 A,H

Structure attributes must be viewed using STN Express query preparation.

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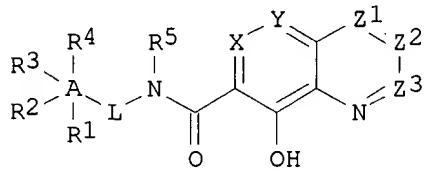
L18 ANSWER 1 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:293652 CAPLUS
DOCUMENT NUMBER: 136:325531
TITLE: Preparation of (poly)azanaphthalenyl carboxamides as HIV integrase inhibitors
INVENTOR(S): Anthony, Neville J.; Gomez, Robert P.; Young, Steven D.; Egbertson, Melissa; Wai, John S.; Zhuang, Linghang; Embrey, Mark; Tran, Lekhanh; Melamed, Jeffrey Y.; Langford, H. Marie; Guare, James P.; Fisher, Thorsten E.; Jolly, Samson M.; Kuo, Michelle S.; Perlow, Debra S.; Bennett, Jennifer J.; Funk, Timothy W.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 434 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002030930	A2	20020418	WO 2001-US31456	20011009
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002011527	A5	20020422	AU 2002-11527	20011009

PRIORITY APPLN. INFO.: US 2000-239707P P 20001012
US 2001-281656P P 20010405
WO 2001-US31456 W 20011009

OTHER SOURCE(S): MARPAT 136:325531
GI



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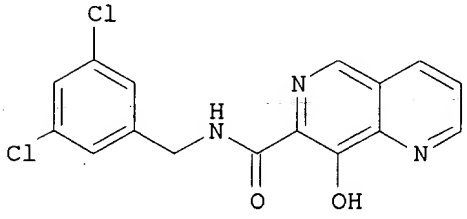


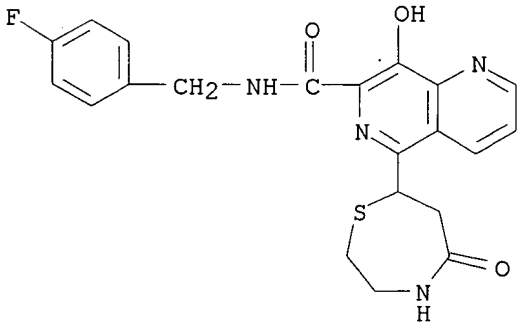
II

AB Title compds., including certain quinoline carboxamide and naphthyridine carboxamide derivs., I [wherein A = (un)substituted Ph or Ph fused to a carbocycle; L = a single bond, or (un)substituted alkyl, alkenyl, alkylcycloalkylalkyl, or alkyl-M-alkyl; M = NRa, OCO, or CO2; X = N or CQ1; Y = N or CQ2, provided that X and Y are not both N; Z1 = N or CQ3; Z2 = N or CQ4; Z3 = N or CH; Q1-Q4 = independently H, halo, CN, NR1CR1O, or (un)substituted alkyl, alkoxy, alkenyl, alkynyl, carbamoyl, carboximidamido, amino, etc.; or C2Q2Q3 = (un)substituted 5- or 6-membered carbocycle or heterocycle; R1 and R2 = independently H, OH, halo, NO2, CN, or (un)substituted alkyl, alkenyl, alkoxy, amino, sulfonylamino, etc.; R3 and R4 = independently H, halo, CN, NO2, OH, alkenyl, or (un)substituted alkyl, amino, sulfonylamino, etc.; R5 = H, CN, CN, or (un)substituted alkyl or aryl; Ra = independently H or (halo)alkyl; or pharmaceutically acceptable salts thereof] were prepd. I are inhibitors of HIV integrase and inhibitors of HIV replication, and are useful in the prevention or treatment of infection by HIV and the treatment of AIDS, as compds. or pharmaceutically acceptable salts, or as ingredients in pharmaceutical compns., optionally in combination with other antivirals, immunomodulators, antibiotics, or vaccines. For example, Mitsunobu reaction of iso-Pr 3-(hydroxymethyl)pyridine-2-carboxylate with Me N-[(4-methylphenyl)sulfonyl]glycinate, followed by cyclization in the presence on NaOMe, afforded Me 8-hydroxy-1,6-naphthyridine-7-carboxylate. Coupling with 3,5-dichlorobenzylamine in toluene gave II. Representative compds. were assayed for the inhibition of acute HIV infection of T-lymphoid cells and demonstrated IC95 values of < 20 .mu.M.

IT **410544-78-4P**, N-(4-Fluorobenzyl)-8-hydroxy-5-(5-oxo-1,4-thiazepan-7-yl)[1,6]naphthyridine-7-carboxamide
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(HIV integrase inhibitor; prepn. of (poly)azanaphthalenyl carboxamides as HIV integrase inhibitors for treatment of AIDS)

RN 410544-78-4 CAPLUS

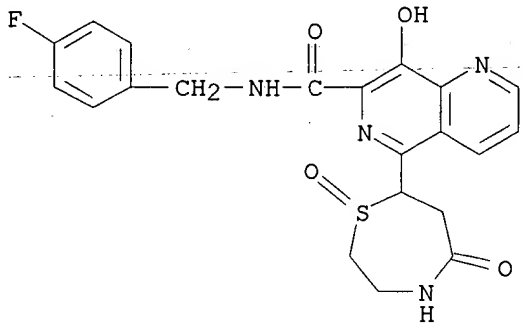
CN 1,6-Naphthyridine-7-carboxamide, N-[(4-fluorophenyl)methyl]-5-(hexahydro-5-oxo-1,4-thiazepin-7-yl)-8-hydroxy- (9CI) (CA INDEX NAME)



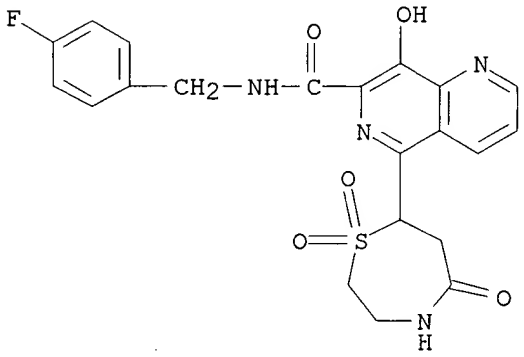
IT **410544-79-5P**, N-(4-Fluorobenzyl)-8-hydroxy-5-(1-oxido-5-oxo-1,4-thiazepan-7-yl)-[1,6]naphthyridine-7-carboxamide **410544-80-8P**, N-(4-Fluorobenzyl)-8-hydroxy-5-(1,1-dioxido-5-oxo-1,4-thiazepan-7-yl)[1,6]-naphthyridine-7-carboxamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(HIV integrase inhibitor; prepn. of (poly)azanaphthalenyl carboxamides as HIV integrase inhibitors for treatment of AIDS)

RN 410544-79-5 CAPLUS
CN 1,6-Naphthyridine-7-carboxamide, N-[(4-fluorophenyl)methyl]-5-(hexahydro-1-oxido-5-oxo-1,4-thiazepin-7-yl)-8-hydroxy- (9CI) (CA INDEX NAME)



RN 410544-80-8 CAPLUS
CN 1,6-Naphthyridine-7-carboxamide, N-[(4-fluorophenyl)methyl]-5-(hexahydro-1,1-dioxido-5-oxo-1,4-thiazepin-7-yl)-8-hydroxy- (9CI) (CA INDEX NAME)

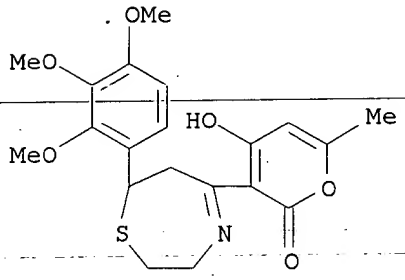


L13 ANSWER 2 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:869523 CAPLUS
DOCUMENT NUMBER: 136:161045
TITLE: Inhibition of P-selectin specific cell adhesion by a low molecular weight, non-carbohydrate compound, KF38789
AUTHOR(S): Ohta, S.; Inujima, Y.; Abe, M.; Uosaki, Y.; Sato, S.; Miki, I.
CORPORATE SOURCE: Department of Immunology, Drug Research Laboratories, Pharmaceutical Research Institute, Kyowa Hakko Kogyo Co., Ltd., Shizuoka, 411-8731, Japan
SOURCE: Inflammation Research (2001), 50(11), 544-551
CODEN: INREFB; ISSN: 1023-3830
PUBLISHER: Birkhaeuser Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English

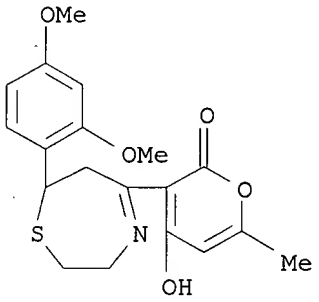
AB Objective and design: P-selectin is a cell adhesion mol. of the selectin family. This study evaluated the effects of novel, low mol. wt. P-selectin inhibitors in a cell adhesion assay and a murine model of peritonitis. Materials: U937 or HL60 was used for cell adhesion assay. Human polymorphonuclear cells were studied for the prodn. of superoxide. BALB/c mice were used for the in vivo study. Treatment: The thioglycollate (TG)-induced accumulation of leukocytes in mice was measured 6 h after the treatment. KF38789 or antibody (1 mg/kg) was injected i.v. prior to TG injection and at 3 h following initial injection. Results: Low mol. wt., non-carbohydrate inhibitors against P-selectin- mediated cell adhesion were tested. One of the most potent inhibitors, KF38789, inhibited the binding of U937 cells to immobilized P-selectin IgG chimeric protein (P-selectin-Ig) with an IC50 value of 1.97 .mu.M. Cell adhesion to both E-selectin-Ig and L-selectin-Ig were not affected even by 100 .mu.M of KF38789. Moreover, KF38789 inhibited P-selectin-induced superoxide prodn. from human polymorphonuclear cells. I.v. injected KF38789 significantly inhibited the TG-induced accumulation of leukocytes in the mouse peritoneal cavity ($p<0.01$). Conclusion: A novel low mol. wt. compd., KF38789, specifically inhibited P-selectin-dependent cell adhesion and the leukocyte recruitment in mouse peritonitis.

IT **257292-28-7 257292-29-8**, KF 38789 **257292-30-1**
257292-31-2 257292-33-4 257292-34-5
257292-36-7 257292-38-9 257292-41-4
257292-44-7
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibition of P-selectin specific cell adhesion by a low mol. wt., non-carbohydrate compd., KF38789)

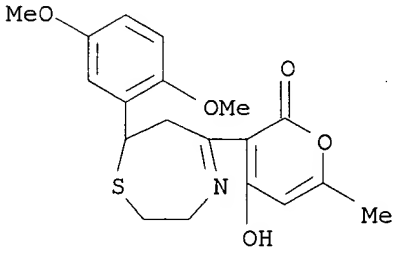
RN 257292-28-7 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2,3,4-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



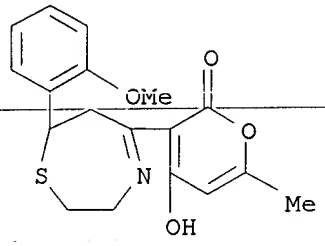
RN 257292-29-8 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



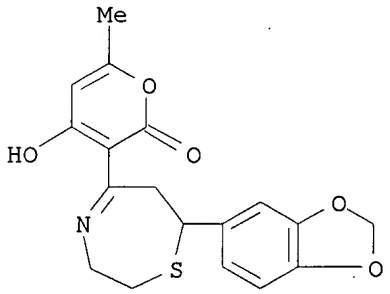
RN 257292-30-1 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,5-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



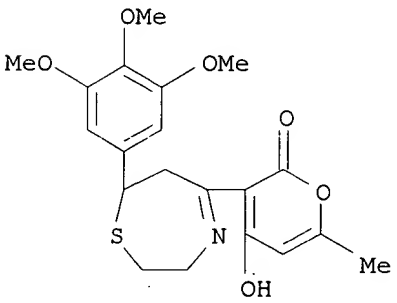
RN 257292-31-2 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



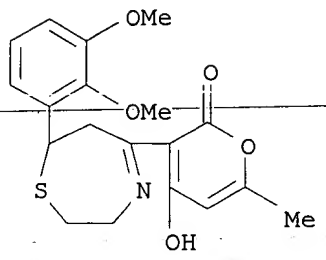
RN 257292-33-4 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(1,3-benzodioxol-5-yl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



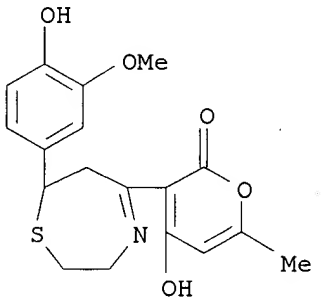
RN 257292-34-5 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(3,4,5-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



RN 257292-36-7 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,3-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



RN 257292-38-9 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(4-hydroxy-3-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



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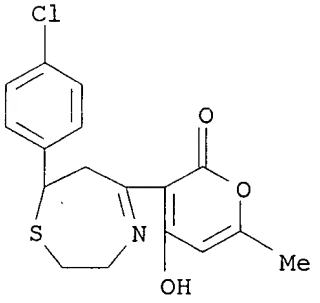
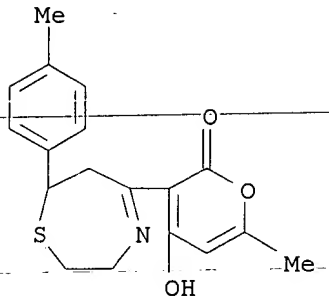
CN 2H-Pyran-2-one, 3-[7-(4-chlorophenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



RN 257292-44-7 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(4-methylphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:780869 CAPLUS
DOCUMENT NUMBER: 135:331449
TITLE: Preparation of substituted 1,4-thiazepines and analogs as activators of caspases and inducers of apoptosis for treatment of cancer and other proliferative diseases
INVENTOR(S): Cai, Sui Xiong; Drewe, John A.; Shelton, Emma Jane; Litvak, Joane; Sperandio, David; Spencer, Jeffrey R.
PATENT ASSIGNEE(S): Cytovia, Inc., USA
SOURCE: PCT Int. Appl., 162 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001079187	A2	20011025	WO 2001-US12581	20010418
WO 2001079187	A3	20020221		
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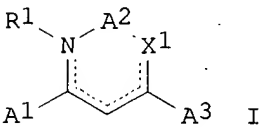
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002010169	A1	20020124	US 2001-836548	20010418

PRIORITY APPLN. INFO.: US 2000-197599P P 20000418
OTHER SOURCE(S): MARPAT 135:331449
GI



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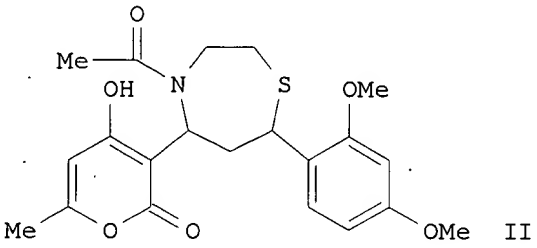


II

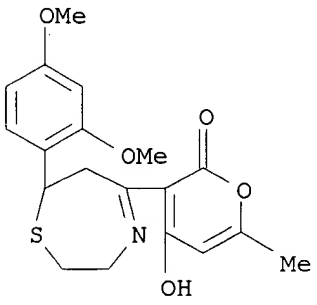
AB Title compds. I [wherein R1 = null, H, alkyl, or COR6; X1 = NR2, S, SO, SO2, or O; R6 = null, H, or (halo)alkyl; A1 = (un)substituted monocyclic or fused polycyclic (hetero)aryl or (hetero)cycloalkyl ring; or A1 and R1 together form an (un)substituted fused polycyclic heteroaryl or heterocycloalkyl ring; the ring contg. A2 = (un)substituted monocyclic or fused bicyclic heteroarylene or heterocycloalkylene ring; A3 = (un)substituted monocyclic or fused polycyclic (hetero)aryl or (hetero)cycloalkyl ring; and N-oxides, prodrugs, protected derivs.,

stereoisomers, and pharmaceutically acceptable salts thereof] were prepd. as caspase activators and apoptosis inducers. For example, coupling of 3-acetyl-4-hydroxy-6-methylpyran-2-one with 2,4-dimethoxybenzaldehyde, followed by cyclization with 2-aminoethanethiol (61%) and acetylation, gave the [1,4]thiazepine II. Five invention compds. were tested and demonstrated caspase potency in human breast cancer cell lines T-47D and ZR-75-1 with EC50 values ranging from 345 nM to 6930 nM and 163 nM to 4207 nM, resp. Thus, I and their compns. with known cancer chemotherapeutic agents are useful for the treatment of drug resistant cancer in animals.

IT **257292-29-8P**, 3-[7-(2,4-Dimethoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of substituted 1,4-thiazepines and analogs as activators of caspases and inducers of apoptosis for treatment of cancer and other proliferative diseases)

RN 257292-29-8 CAPLUS

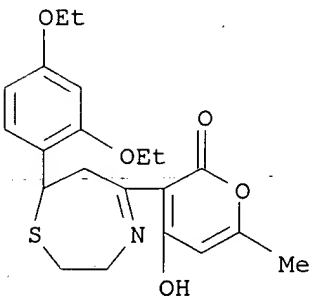
CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



IT **369388-77-2P**, 4-Hydroxy-3-[7-(2,4-diethoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-6-methylpyran-2-one
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of substituted 1,4-thiazepines and analogs as activators of caspases and inducers of apoptosis for treatment of cancer and other proliferative diseases)

RN 369388-77-2 CAPLUS

CN 2H-Pyran-2-one, 3-[7-(2,4-diethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)

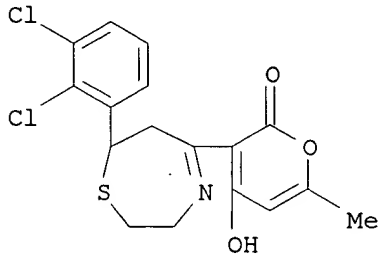


IT **331852-70-1P**, 3-[7-(2,3-Dichlorophenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]4-hydroxy-6-methylpyran-2-one **331857-68-2P**, 4-Hydroxy-6-methyl-3-[7-(4-methylthiophenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one **331857-79-5P**, 3-[7-(4-Ethoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **331857-86-4P**, 3-[7-(2-Bromophenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]4-hydroxy-6-methylpyran-2-one **369387-63-3P**, 4-Hydroxy-6-methyl-3-[7-(3-phenyl-1H-pyrazol-4-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one **369387-65-5P**, 3-[7-(5-Ethylthien-2-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369387-66-6P**, 3-[7-(1-Benzyl-1H-indol-3-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369387-68-8P**, 4-Hydroxy-6-methyl-3-[7-(2-trifluoromethylthiophenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one **369387-69-9P**, 4-Hydroxy-6-methyl-3-[7-(3-trifluoromethylthiophenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one **369387-71-3P**, 4-Hydroxy-6-methyl-3-[7-(4-trifluoromethylthiophenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one **369387-72-4P**, 4-Hydroxy-6-methyl-3-[7-[3-(3-trifluoromethylphenoxy)phenyl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one **369387-74-6P**, 3-[7-[3-(3,4-Dichlorophenoxy)phenyl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369387-76-8P**, 3-[7-[3-(3,5-Dichlorophenoxy)phenyl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369387-77-9P**, 4-Hydroxy-6-methyl-3-[7-[5-(3-trifluoromethylphenyl)furan-2-yl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one **369387-79-1P**, 3-[7-[5-(2-Chlorophenyl)furan-2-yl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369387-80-4P**, 3-[7-[5-(3-Chlorophenyl)furan-2-yl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369387-81-5P**, 3-[7-[5-(4-Chlorophenyl)furan-2-yl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369387-82-6P**, 4-Hydroxy-6-methyl-3-[7-[5-(2-chloro-5-trifluoromethylphenyl)furan-2-yl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one **369387-83-7P**, 3-[7-(4-Bromothien-2-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369387-84-8P**, 3-[7-(5-Bromothien-2-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369387-86-0P**, 3-[7-(1-Benzylsulfonyl-1H-pyrrol-2-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369387-88-2P**, 4-Hydroxy-6-methyl-3-[7-(3-methylthien-2-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one **369387-89-3P**, 4-Hydroxy-6-methyl-3-[7-(5-methylthien-2-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one **369387-91-7P**, 4-Hydroxy-6-methyl-3-[7-(1-methyl-1H-indol-3-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one **369387-93-9P**, 3-[7-(3-Chloro-2-methyl-5-trifluoromethyl-1H-pyrazol-4-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369387-94-0P**, 3-[7-[1-(2,4-Difluorobenzylsulfonyl)-1H-pyrrol-2-yl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369387-96-2P**, 3-(7-[2,2']Bithienyl-5-yl-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl)-4-hydroxy-6-methylpyran-2-one **369387-97-3P**, 3-[7-[1-(3,5-Dichlorophenyl)-1H-pyrrol-2-yl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369387-99-5P**, 3-[7-[1-(4-Chlorophenyl)-1H-pyrrol-2-yl]-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369388-00-1P** **369388-03-4P**, 4-Hydroxy-6-methyl-3-[7-(6-p-tolylthioimidazo[2,1-

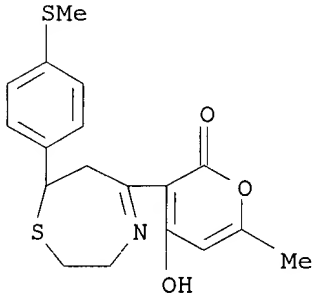
b]thiazol-5-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one **369388-06-7P**, 3-[7-(4,5-Dibromothien-2-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369388-09-0P**, 4-Hydroxy-6-methyl-3-[7-(5-methylthiothien-2-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one **369388-12-5P**, 3-[7-(5-Chloro-1-methyl-3-phenyl-1H-pyrazol-4-yl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369388-14-7P**, 3-[7-(4-Dimethylaminophenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369388-15-8P**, 4-Hydroxy-6-methyl-3-[7-(4-trifluoromethoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one **369388-17-0P**, 4-Hydroxy-3-[7-(4-methylsulfonylphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-6-methylpyran-2-one **369388-19-2P**, 3-[7-(2,4-Dimethoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-methoxy-6-methylpyran-2-one **369388-21-6P**, 3-[7-(2,4-Dimethoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methyl-5,6-dihydropyran-2-one **369388-23-8P**, 3-[7-(2,4-Diethoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methyl-5,6-dihydropyran-2-one **369388-25-0P**, 3-[7-(4-Dimethylaminophenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methyl-5,6-dihydropyran-2-one **369388-27-2P**, 3-[7-(2,3,4-Trimethoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methyl-5,6-dihydropyran-2-one **369388-29-4P** **369388-31-8P** **369388-33-0P** **369388-35-2P**, 3-[7-(2,4-Dimethoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-1H-quinolin-2-one **369388-44-3P**, 3-[4-Acetyl-7-(2,4-dimethoxyphenyl)[1,4]thiazepan-5-yl]-4-hydroxy-6-methylpyran-2-one **369388-46-5P**, 3-[7-(2,4-Dimethoxyphenyl)-4-(2,2,2-trifluoroethanoyl)-[1,4]thiazepan-5-yl]-4-hydroxy-6-methylpyran-2-one **369388-48-7P**, 1-[7-(2,4-Dimethoxyphenyl)-5-(3-fluoro-4-methoxyphenyl)-[1,4]thiazepan-4-yl]ethanone **369388-50-1P**, 3-[7-(2,4-Dimethoxyphenyl)-2,3-dihydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369388-52-3P**, 3-[7-(2,4-Diethoxyphenyl)-2,3-dihydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369388-54-5P** **369388-56-7P**, 3-[7-(2,4-Diethoxyphenyl)-2,3-dihydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methyl-5,6-dihydropyran-2-one **369388-58-9P** **369388-60-3P**, 3-[7-(2,4-Dimethoxyphenyl)-1-oxo-2,3,6,7-tetrahydro-1H-1.lambda.4-[1,4]thiazepin-5-yl]-4-hydroxy-6-methoxypyran-2-one **369388-62-5P** **369388-67-0P**, 10-(2,4-Dimethoxyphenyl)-3-methyl-7,8-dihydro-10H-2,5-dioxa-9-thia-6a-azacyclohepta[a]naphthalene-1,6-dione **369388-69-2P**, 4-Hydroxy-3-[7-(2-methoxy-4-methylthiophenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-6-methylpyran-2-one **369388-71-6P**, 3-[7-(2-Chloro-5-trifluoromethylphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369388-73-8P**, 3-[7-(4-Dimethylamino-2-methoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369388-75-0P**, 4-Hydroxy-3-[7-(4-chloro-2-methoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-6-methylpyran-2-one **369388-79-4P**, 7-(2,4-Dimethoxyphenyl)-5-(4-hydroxy-6-methyl-2-oxo-2H-pyran-3-yl)-2,2-dimethyl-2,3,6,7-tetrahydro-[1,4]thiazepine-3-carboxylic acid **369388-81-8P** **369388-85-2P**, 3-[7-(3-Methoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-6-methylpyran-2-one **369388-89-6P**, 3-[7-(3,4-Dichlorophenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369388-91-0P**, 6-Methyl-3-[7-(2,3,4-trimethoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one **369389-71-9P**, 3-[7-(2,4-Dimethoxyphenyl)-1-oxo-2,3,6,7-tetrahydro-1H-1.lambda.4-[1,4]thiazepin-5-yl]-4-hydroxy-6-methylpyran-2-one **369389-72-0P**, 4-Hydroxy-6-methyl-3-[7-(3-

methoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepin-5-yl]pyran-2-one
369605-23-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of substituted 1,4-thiazepines and analogs as activators of caspases and inducers of apoptosis for treatment of cancer and other proliferative diseases)

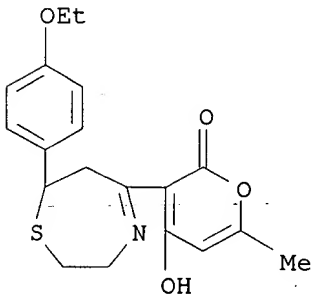
RN 331852-70-1 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,3-dichlorophenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



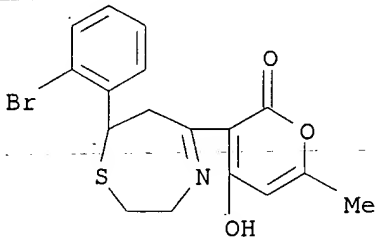
RN 331857-68-2 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[4-(methylthio)phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



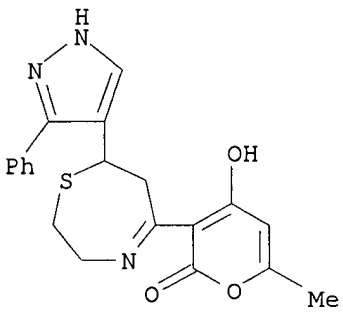
RN 331857-79-5 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(4-ethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



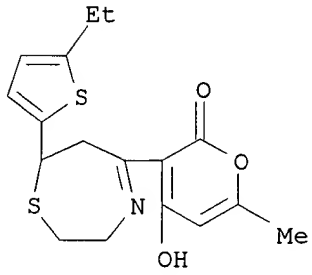
RN 331857-86-4 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2-bromophenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



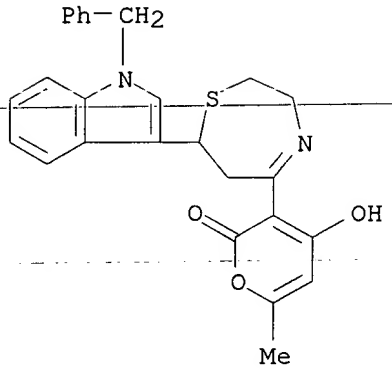
RN 369387-63-3 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(3-phenyl-1H-pyrazol-4-yl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



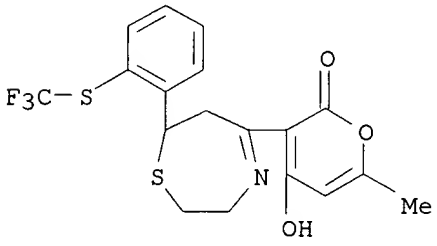
RN 369387-65-5 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(5-ethyl-2-thienyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



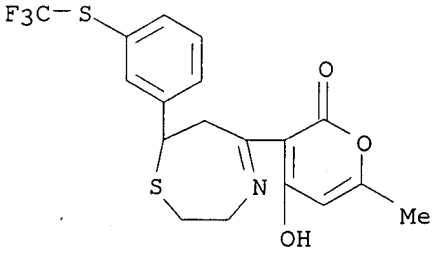
RN 369387-66-6 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[1-(phenylmethyl)-1H-indol-3-yl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



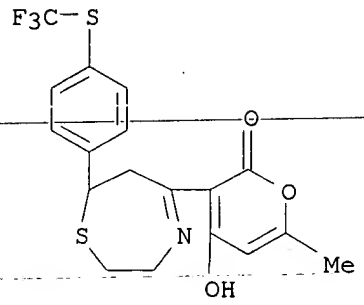
RN 369387-68-8 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[2-[(trifluoromethyl)thio]phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



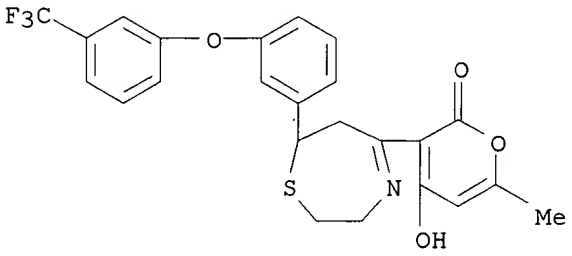
RN 369387-69-9 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[3-[(trifluoromethyl)thio]phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



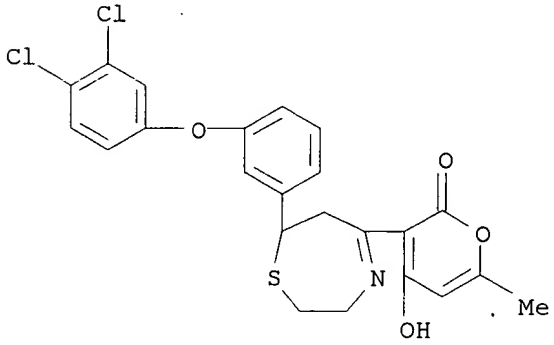
RN 369387-71-3 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[4-[(trifluoromethyl)thio]phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



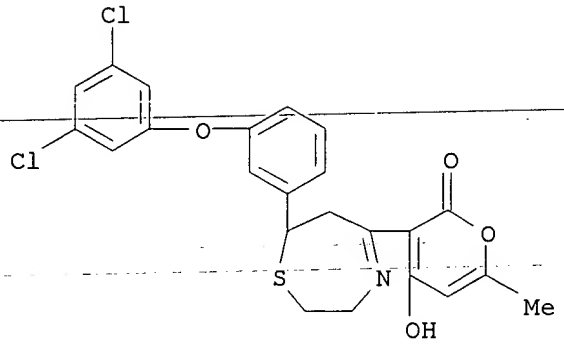
RN 369387-72-4 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[3-[3-(trifluoromethyl)phenoxy]phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



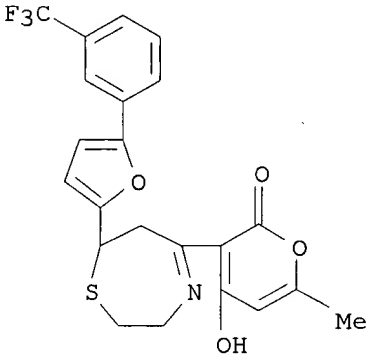
RN 369387-74-6 CAPLUS
CN 2H-Pyran-2-one, 3-[7-[3-(3,4-dichlorophenoxy)phenyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



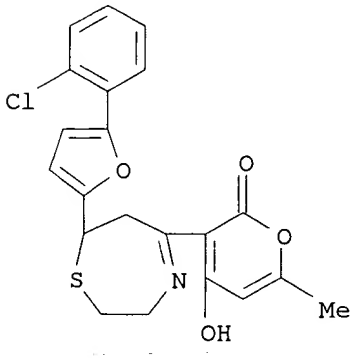
RN 369387-76-8 CAPLUS
CN 2H-Pyran-2-one, 3-[7-[3-(3,5-dichlorophenoxy)phenyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



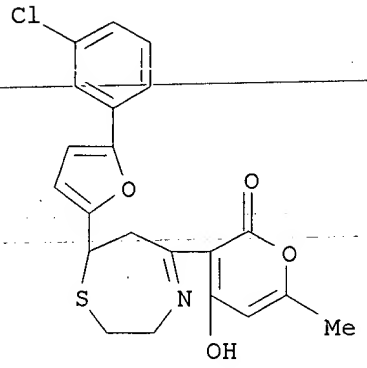
RN 369387-77-9 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[5-[3-(trifluoromethyl)phenyl]-2-furanyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



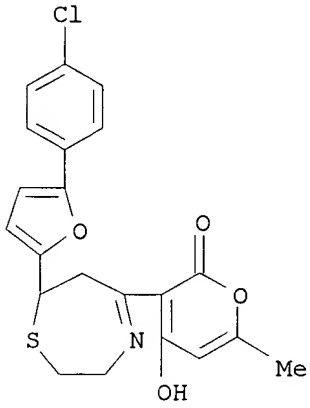
RN 369387-79-1 CAPLUS
CN 2H-Pyran-2-one, 3-[7-[5-(2-chlorophenyl)-2-furanyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



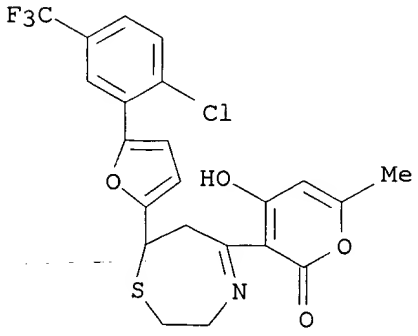
RN 369387-80-4 CAPLUS
CN 2H-Pyran-2-one, 3-[7-[5-(3-chlorophenyl)-2-furanyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



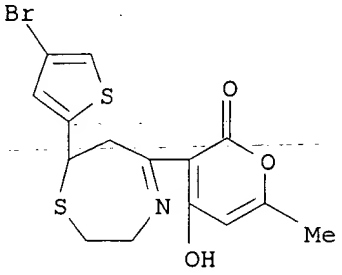
RN 369387-81-5 CAPLUS
CN 2H-Pyran-2-one, 3-[7-[5-(4-chlorophenyl)-2-furanyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



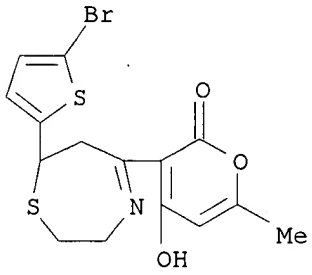
RN 369387-82-6 CAPLUS
CN 2H-Pyran-2-one, 3-[7-[5-[2-chloro-5-(trifluoromethyl)phenyl]-2-furanyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



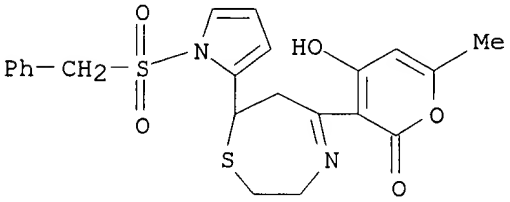
RN 369387-83-7 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(4-bromo-2-thienyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



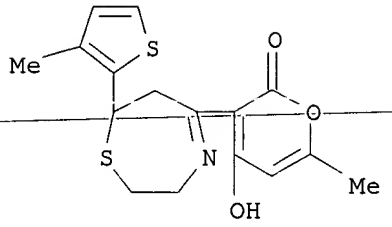
RN 369387-84-8 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(5-bromo-2-thienyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



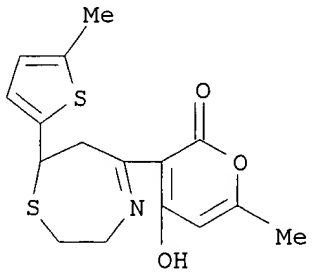
RN 369387-86-0 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[1-[(phenylmethyl)sulfonyl]-1H-pyrrol-2-yl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



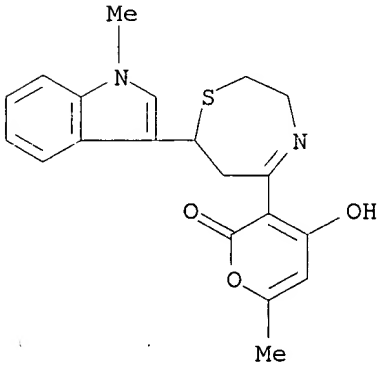
RN 369387-88-2 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(3-methyl-2-thienyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



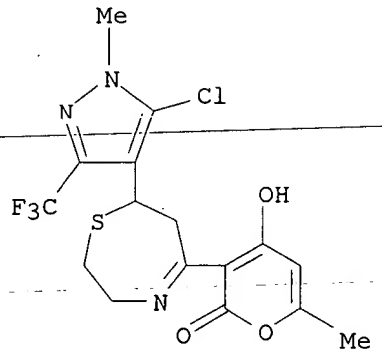
RN 369387-89-3 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(5-methyl-2-thienyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



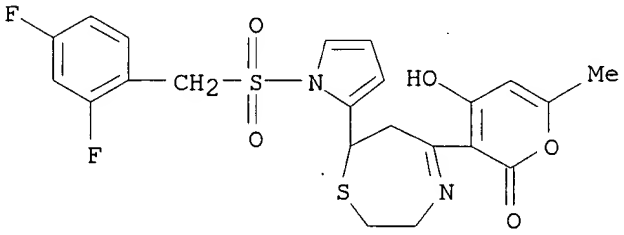
RN 369387-91-7 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(1-methyl-1H-indol-3-yl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



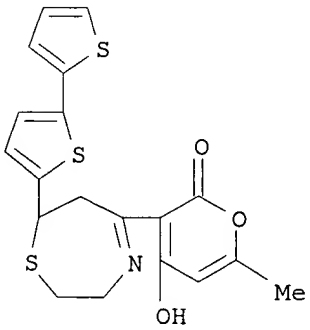
RN 369387-93-9 CAPLUS
CN 2H-Pyran-2-one, 3-[7-[5-chloro-1-methyl-3-(trifluoromethyl)-1H-pyrazol-4-yl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



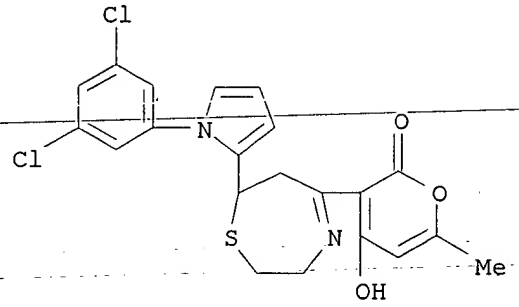
RN 369387-94-0 CAPLUS
CN 2H-Pyran-2-one, 3-[7-[1-[[(2,4-difluorophenyl)methyl]sulfonyl]-1H-pyrrol-2-yl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



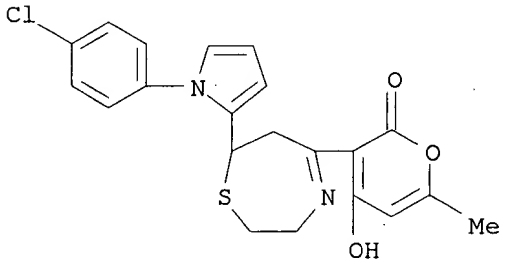
RN 369387-96-2 CAPLUS
CN 2H-Pyran-2-one, 3-(7-[2,2'-bithiophen]-5-yl-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl)-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



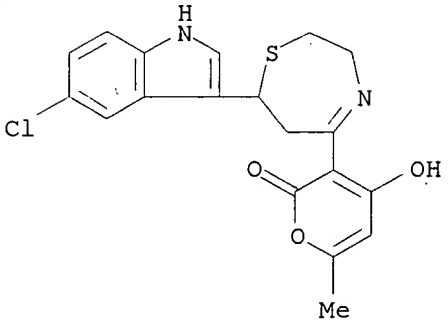
RN 369387-97-3 CAPLUS
CN 2H-Pyran-2-one, 3-[7-[1-(3,5-dichlorophenyl)-1H-pyrrol-2-yl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



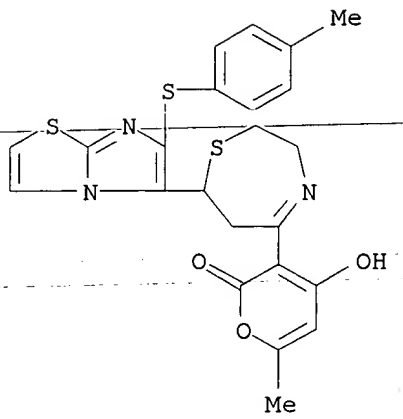
RN 369387-99-5 CAPLUS
CN 2H-Pyran-2-one, 3-[7-[1-(4-chlorophenyl)-1H-pyrrol-2-yl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



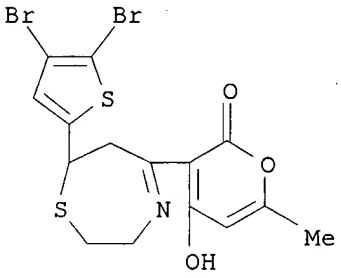
RN 369388-00-1 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(5-chloro-1H-indol-3-yl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



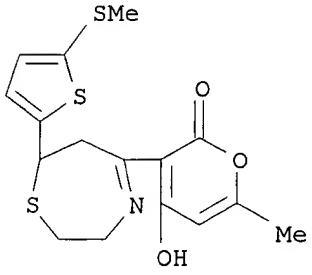
RN 369388-03-4 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[6-[(4-methylphenyl)thio]imidazo[2,1-b]thiazol-5-yl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



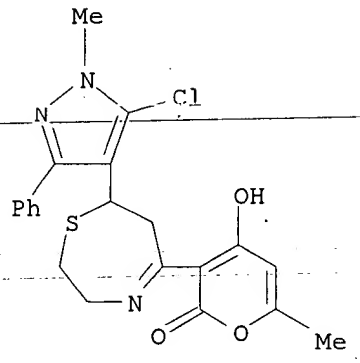
RN 369388-06-7 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(4,5-dibromo-2-thienyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



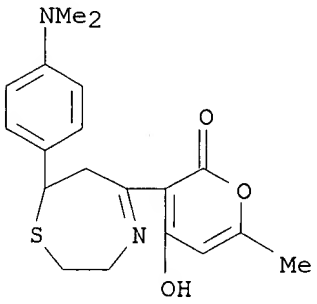
RN 369388-09-0 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[5-(methylthio)-2-thienyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



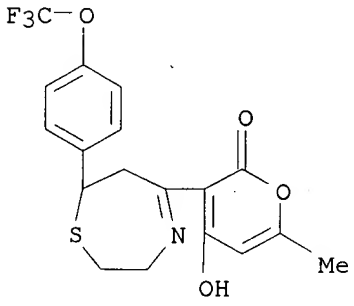
RN 369388-12-5 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(5-chloro-1-methyl-3-phenyl-1H-pyrazol-4-yl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



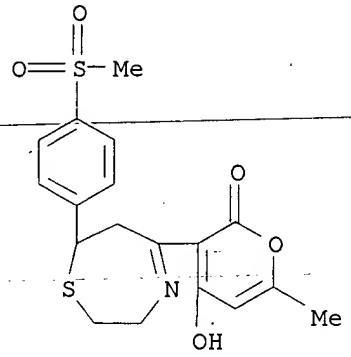
RN 369388-14-7 CAPLUS
CN 2H-Pyran-2-one, 3-[7-[4-(dimethylamino)phenyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



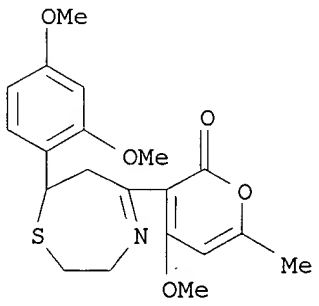
RN 369388-15-8 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[4-(trifluoromethoxy)phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



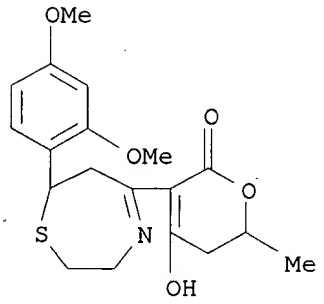
RN 369388-17-0 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[4-(methylsulfonyl)phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



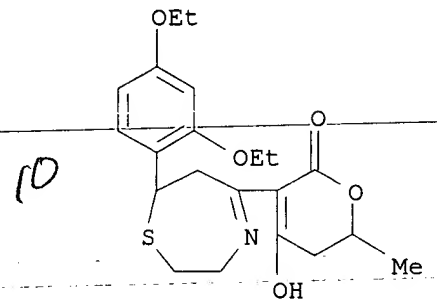
RN 369388-19-2 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-methoxy-6-methyl- (9CI) (CA INDEX NAME)



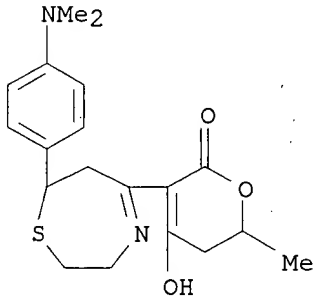
RN 369388-21-6 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-5,6-dihydro-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



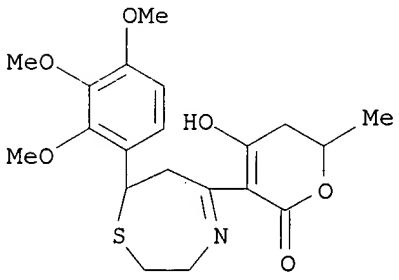
RN 369388-23-8 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,4-diethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-5,6-dihydro-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



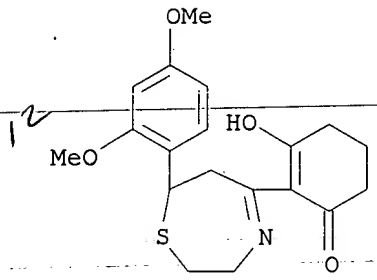
RN 369388-25-0 CAPLUS
CN 2H-Pyran-2-one, 3-[7-[4-(dimethylamino)phenyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-5,6-dihydro-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



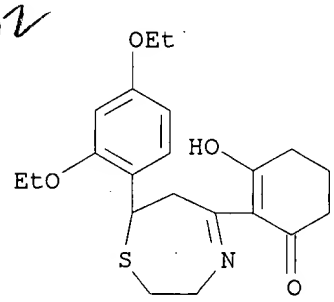
RN 369388-27-2 CAPLUS
CN 2H-Pyran-2-one, 5,6-dihydro-4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2,3,4-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



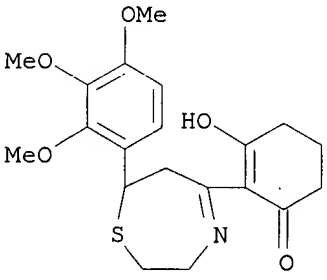
RN 369388-29-4 CAPLUS
CN 2-Cyclohexen-1-one, 2-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-3-hydroxy- (9CI) (CA INDEX NAME)



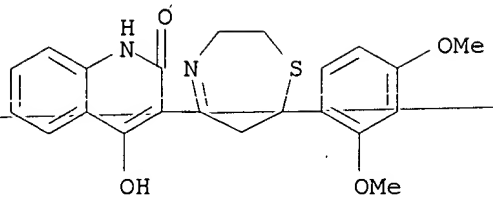
RN 369388-31-8 CAPLUS
CN 2-Cyclohexen-1-one, 2-[7-(2,4-diethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-3-hydroxy- (9CI) (CA INDEX NAME)



RN 369388-33-0 CAPLUS
CN 2-Cyclohexen-1-one, 3-hydroxy-2-[2,3,6,7-tetrahydro-7-(2,3,4-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



RN 369388-35-2 CAPLUS
CN 2(1H)-Quinolinone, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy- (9CI) (CA INDEX NAME)



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RN 369388-44-3 CAPLUS
CN 1,4-Thiazepine, 4-acetyl-7-(2,4-dimethoxyphenyl)hexahydro-5-(4-hydroxy-6-methyl-2-oxo-2H-pyran-3-yl)- (9CI) (CA INDEX NAME)

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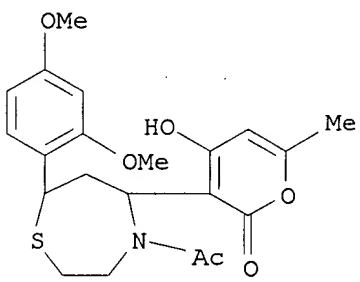

RN 369388-46-5 CAPLUS
CN 1,4-Thiazepine, 7-(2,4-dimethoxyphenyl)hexahydro-5-(4-hydroxy-6-methyl-2-oxo-2H-pyran-3-yl)-4-(trifluoroacetyl)- (9CI) (CA INDEX NAME)

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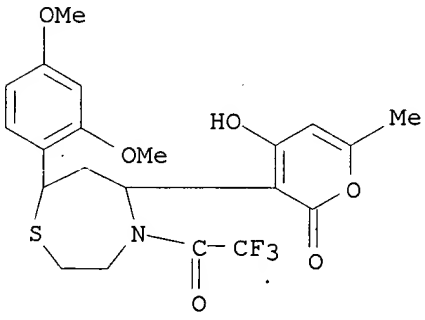
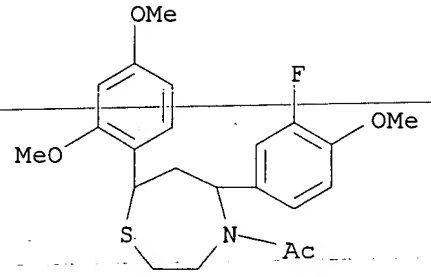


RN 369388-48-7 CAPLUS
CN 1,4-Thiazepine, 4-acetyl-7-(2,4-dimethoxyphenyl)-5-(3-fluoro-4-methoxyphenyl)hexahydro- (9CI) (CA INDEX NAME)



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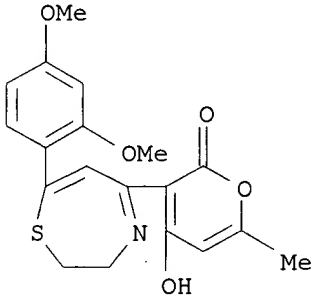
RN 369388-50-1 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3-dihydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



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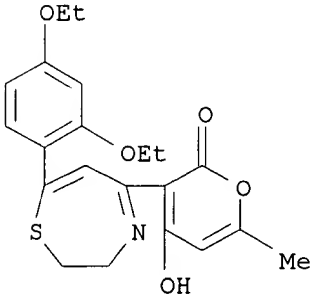
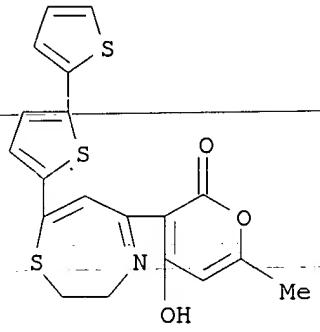
RN 369388-52-3 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,4-diethoxyphenyl)-2,3-dihydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



30

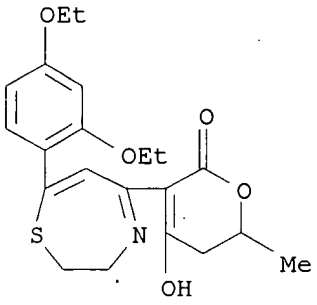
RN 369388-54-5 CAPLUS
CN 2H-Pyran-2-one, 3-(7-[2,2'-bithiophen]-5-yl-2,3-dihydro-1,4-thiazepin-5-yl)-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)

30



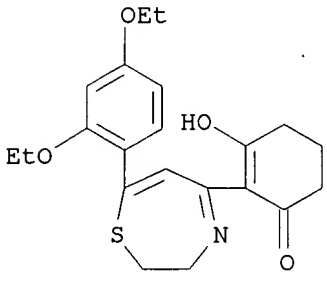
RN 369388-56-7 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,4-diethoxyphenyl)-2,3-dihydro-1,4-thiazepin-5-yl]-5,6-dihydro-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)

32

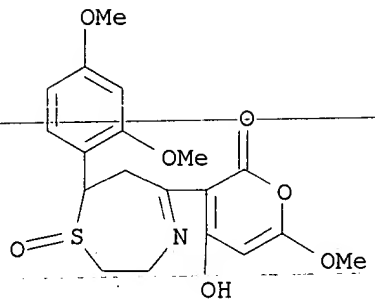


RN 369388-58-9 CAPLUS
CN 2-Cyclohexen-1-one, 2-[7-(2,4-diethoxyphenyl)-2,3-dihydro-1,4-thiazepin-5-yl]-3-hydroxy- (9CI) (CA INDEX NAME)

34

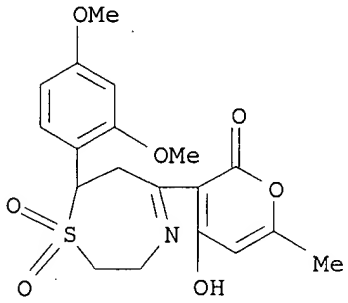


RN 369388-60-3 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1-oxido-1,4-thiazepin-5-yl]-4-hydroxy-6-methoxy- (9CI) (CA INDEX NAME)



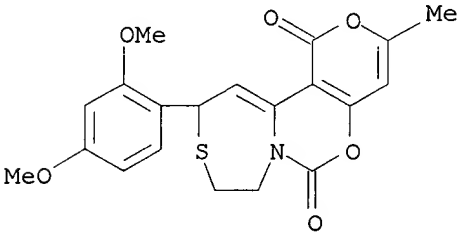
38

RN 369388-62-5 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,1-dioxido-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)

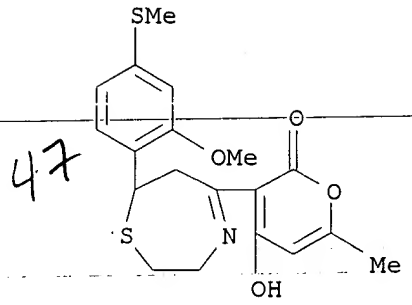


40

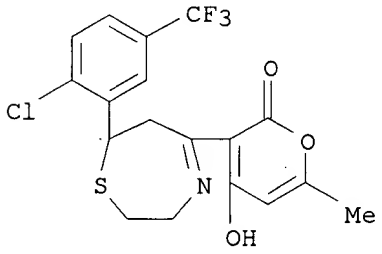
RN 369388-67-0 CAPLUS
CN 1H,6H,11H-Pyrano[3',4':5,6][1,3]oxazino[3,4-d][1,4]thiazepine-1,6-dione, 11-(2,4-dimethoxyphenyl)-8,9-dihydro-3-methyl- (9CI) (CA INDEX NAME)



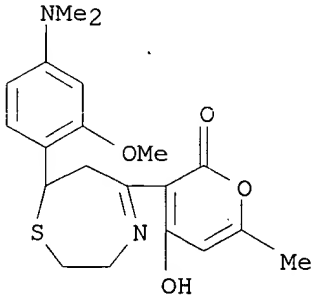
RN 369388-69-2 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[2-methoxy-4-(methylthio)phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



RN 369388-71-6 CAPLUS
CN 2H-Pyran-2-one, 3-[7-[2-chloro-5-(trifluoromethyl)phenyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)

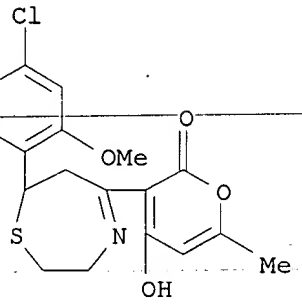


RN 369388-73-8 CAPLUS
CN 2H-Pyran-2-one, 3-[7-[4-(dimethylamino)-2-methoxyphenyl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



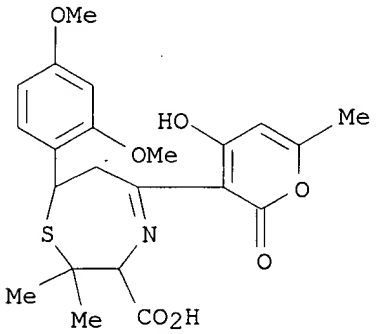
RN 369388-75-0 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(4-chloro-2-methoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)

47



RN 369388-79-4 CAPLUS
CN 1,4-Thiazepine-3-carboxylic acid, 7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-5-(4-hydroxy-6-methyl-2-oxo-2H-pyran-3-yl)-2,2-dimethyl- (9CI) (CA INDEX NAME)

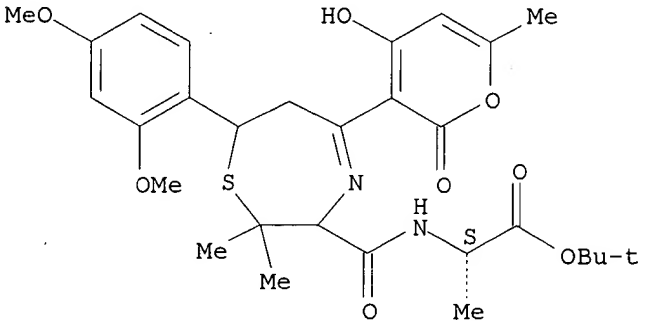
48



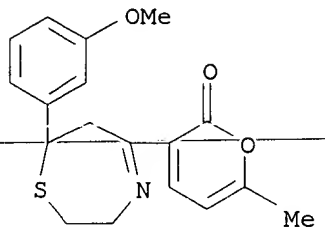
RN 369388-81-8 CAPLUS
CN L-Alanine, N-[[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-5-(4-hydroxy-6-methyl-2-oxo-2H-pyran-3-yl)-2,2-dimethyl-1,4-thiazepin-3-yl]carbonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

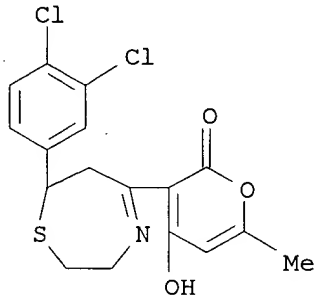
48



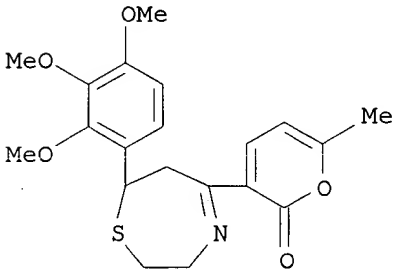
RN 369388-85-2 CAPLUS
CN 2H-Pyran-2-one, 6-methyl-3-[2,3,6,7-tetrahydro-7-(3-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



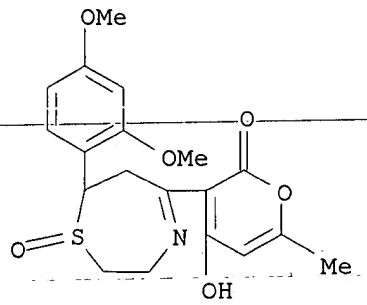
RN 369388-89-6 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(3,4-dichlorophenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



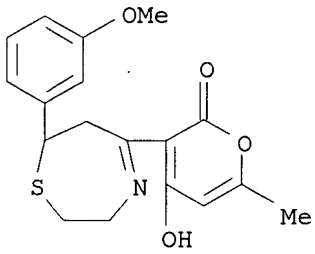
RN 369388-91-0 CAPLUS
CN 2H-Pyran-2-one, 6-methyl-3-[2,3,6,7-tetrahydro-7-(2,3,4-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



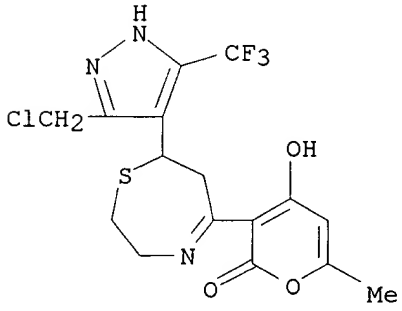
RN 369389-71-9 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1-oxido-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



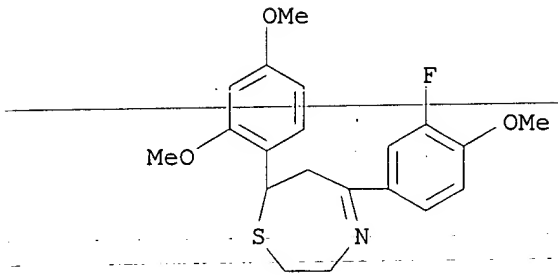
RN 369389-72-0 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(3-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



RN 369605-23-2 CAPLUS
CN 2H-Pyran-2-one, 3-[7-[3-(chloromethyl)-5-(trifluoromethyl)-1H-pyrazol-4-yl]-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



IT **369389-06-0**, 7-(2,4-Dimethoxyphenyl)-5-(3-fluoro-4-methoxyphenyl)-2,3,6,7-tetrahydro-[1,4]thiazepine
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; prepn. of substituted 1,4-thiazepines and analogs as activators of caspases and inducers of apoptosis for treatment of cancer and other proliferative diseases)
RN 369389-06-0 CAPLUS
CN 1,4-Thiazepine, 7-(2,4-dimethoxyphenyl)-5-(3-fluoro-4-methoxyphenyl)-2,3,6,7-tetrahydro- (9CI) (CA INDEX NAME)


OMe
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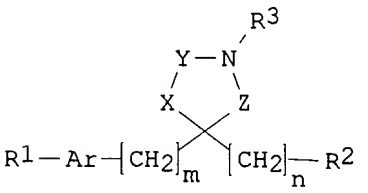
L13 ANSWER 4 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:617988 CAPLUS
DOCUMENT NUMBER: 135:195581
TITLE: Preparation of thiazepinyl hydroxamic acid derivatives as matrix metalloproteinase inhibitors
INVENTOR(S): Neya, Masahiro; Yamazaki, Hitoshi; Ohne, Kazuhiko; Sawada, Yuki; Mizutani, Tsuyoshi; Imamura, Yoshimasa; Mukai, Noriko
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 446 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

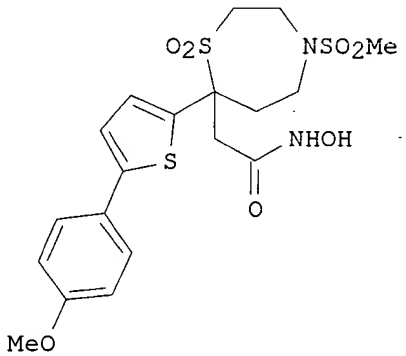
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001060808	A1	20010823	WO 2001-JP1206	20010220

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: AU 2000-5751 A 20000221
AU 2000-8603 A 20000706
OTHER SOURCE(S): MARPAT 135:195581
GI



I

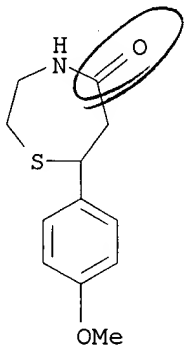


II

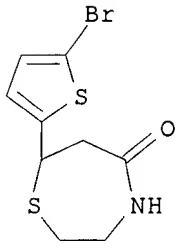
AB The title compds. [I; R1 = halo, alkoxy, (un)substituted aryl, etc.; R2 = amidated carboxy; R3 = H, acyl; Ar = aryl, heterocyclyl; X = S, SO, SO2; Y, Z = alkylene; m, n = 0-2], useful as inhibitors of matrix metalloproteinases (MMP) or the prodn. of tumor necrosis factor .alpha. (TNF .alpha.), were prepd. E.g., a multi-step synthesis of II which showed IC50 of 2.85 nM against human MMP-9, was given.

IT **73920-60-2P 355849-35-3P 355849-50-2P**
355850-10-1P 355850-16-7P 355850-22-5P
355850-62-3P 355850-82-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of thiazepinyl hydroxamic acid derivs. as matrix metalloproteinase inhibitors)

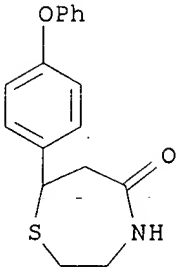
RN 73920-60-2 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



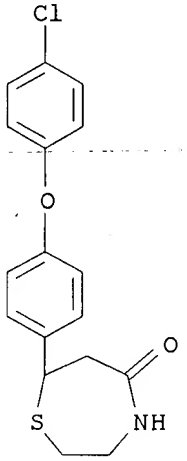
RN 355849-35-3 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, 7-(5-bromo-2-thienyl)tetrahydro- (9CI) (CA INDEX NAME)



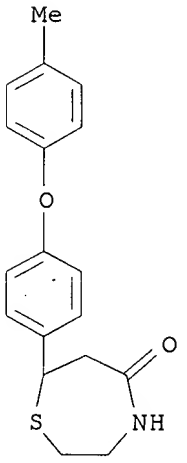
RN 355849-50-2 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME)



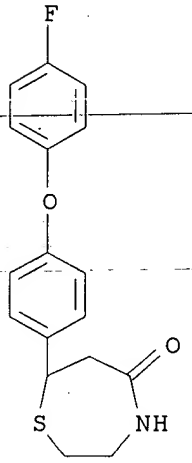
RN 355850-10-1 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, 7-[4-(4-chlorophenoxy)phenyl]tetrahydro- (9CI) (CA INDEX NAME)



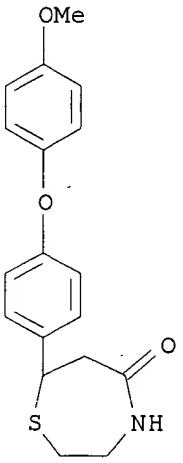
RN 355850-16-7 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-[4-(4-methylphenoxy)phenyl]- (9CI) (CA INDEX NAME)



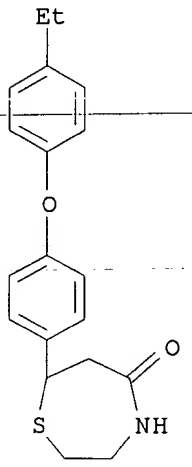
RN 355850-22-5 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, 7-[4-(4-fluorophenoxy)phenyl]tetrahydro- (9CI) (CA INDEX NAME)



RN 355850-62-3 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-[4-(4-methoxyphenoxy)phenyl]- (9CI) (CA INDEX NAME)



RN 355850-82-7 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, 7-[4-(4-ethylphenoxy)phenyl]tetrahydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

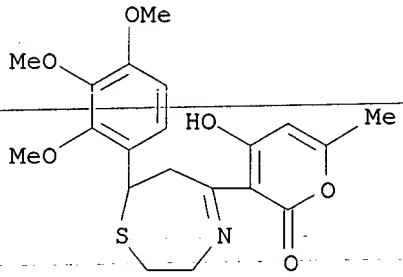
L13 ANSWER 5 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:258482 CAPLUS
DOCUMENT NUMBER: 133:117069
TITLE: Dissecting cellular processes using small molecules: identification of colchicine-like, taxol-like and other small molecules that perturb mitosis
AUTHOR(S): Haggarty, Stephen J.; Mayer, Thomas U.; Miyamoto, David T.; Fathi, Reza; King, Randall W.; Mitchison, Timothy J.; Schreiber, Stuart L.
CORPORATE SOURCE: Harvard Institute of Chemistry and Cell Biology, Harvard Medical School, Boston, MA, 02115, USA
SOURCE: Chemistry & Biology (2000), 7(4), 275-286
CODEN: CBOLE2; ISSN: 1074-5521
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

April

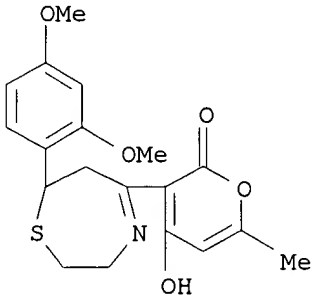
AB Background: Understanding the mol. mechanisms of complex cellular processes requires unbiased means to identify and to alter conditionally gene products that function in a pathway of interest. Although random mutagenesis and screening (forward genetics) provide a useful means to this end, the complexity of the genome, long generation time and redundancy of gene function have limited their use with mammalian systems. We sought to develop an analogous process using small mols. to modulate conditionally the function of proteins. We hoped to identify simultaneously small mols. that may serve as leads for the development of therapeutically useful agents. Results: We report the results of a high-throughput, phenotype-based screen for identifying cell-permeable small mols. that affect mitosis of mammalian cells. The predominant class of compds. that emerged directly alters the stability of microtubules in the mitotic spindle. Although many of these compds. show the colchicine-like property of destabilizing microtubules, one member shows the taxol-like property of stabilizing microtubules. Another class of compds. alters chromosome segregation by novel mechanisms that do not involve direct interactions with microtubules. Conclusions: The identification of structurally diverse small mols. that affect the mammalian mitotic machinery from a large library of synthetic compds. illustrates the use of chem. genetics in dissecting an essential cellular pathway. This screen identified five compds. that affect mitosis without directly targeting microtubules. Understanding the mechanism of action of these compds., along with future screening efforts, promises to help elucidate the mol. mechanisms involved in chromosome segregation during mitosis.

IT **257292-28-7 257292-29-8 257292-30-1**
257292-31-2 257292-32-3 257292-33-4
257292-34-5 257292-35-6 257292-36-7
257292-37-8 257292-38-9 257292-39-0
257292-40-3 257292-41-4 257292-42-5
257292-43-6 257292-44-7
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(phenotype-based screening of compd. library to identify cell-permeable small mols. that affect mitosis of mammalian cells)

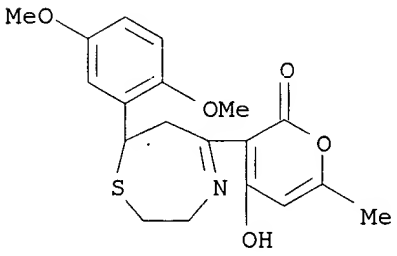
RN 257292-28-7 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2,3,4-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



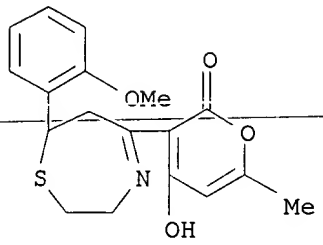
RN 257292-29-8 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



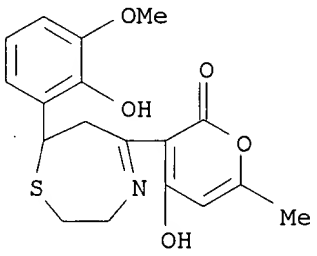
RN 257292-30-1 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,5-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



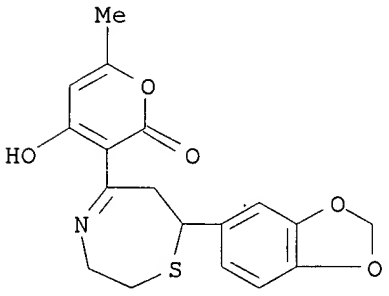
RN 257292-31-2 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



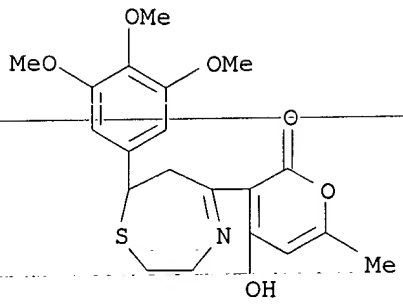
RN 257292-32-3 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2-hydroxy-3-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



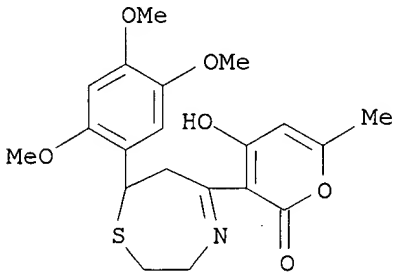
RN 257292-33-4 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(1,3-benzodioxol-5-yl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



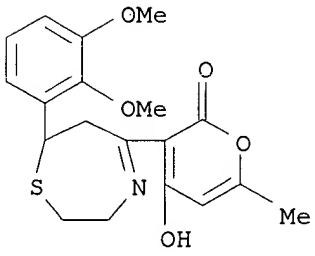
RN 257292-34-5 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(3,4,5-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



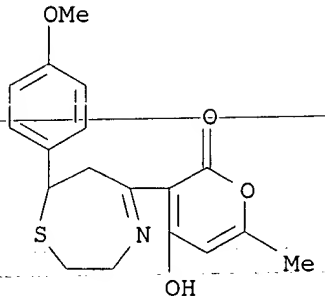
RN 257292-35-6 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2,4,5-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



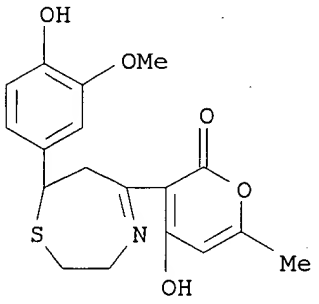
RN 257292-36-7 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,3-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



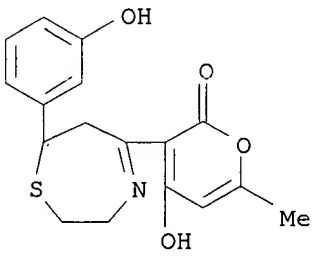
RN 257292-37-8 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(4-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



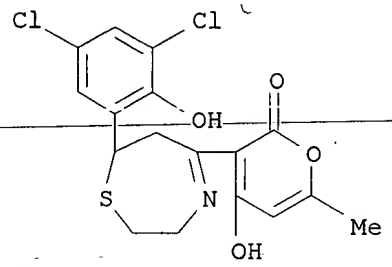
RN 257292-38-9 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(4-hydroxy-3-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



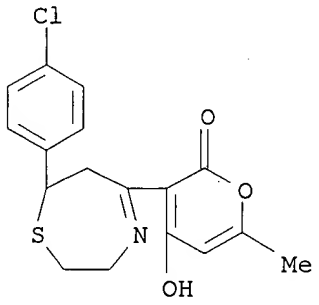
RN 257292-39-0 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(3-hydroxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



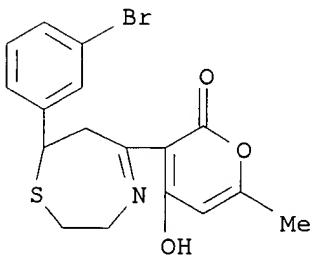
RN 257292-40-3 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(3,5-dichloro-2-hydroxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



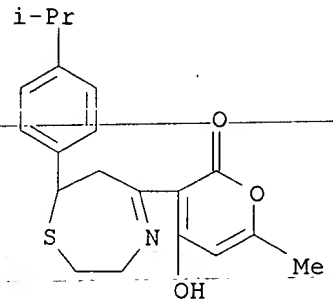
RN 257292-41-4 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(4-chlorophenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



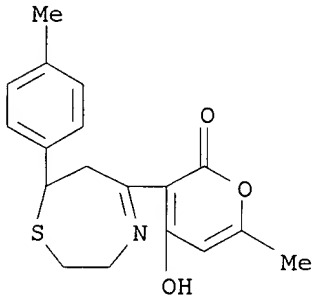
RN 257292-42-5 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(3-bromophenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



RN 257292-43-6 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[4-(1-methylethyl)phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



RN 257292-44-7 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(4-methylphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

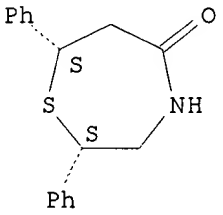
L13 ANSWER 6 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:148732 CAPLUS
DOCUMENT NUMBER: 132:293716
TITLE: Tetrahydrothiapyran-4-ones. Source for annelated 1,2,3-selena/thiadiazoles and their reactivity
AUTHOR(S): Reddy, D. Bhaskar; Reddy, A. Somasekhar; Reddy, N. Subba
CORPORATE SOURCE: Department of Chemistry, Sri Venkateswara University, Tirupati, 517 502, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1999), 38B(12), 1342-1348
CODEN: IJSBDB; ISSN: 0376-4699
PUBLISHER: National Institute of Science Communication, CSIR
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:293716

AB 1,2,3-Selenadiazole and 1,2,3-thiadiazole rings were fused to 2,6-diaryl-(3-alkyl)-tetrahydrothiapyran-4-ones (I) utilizing an .alpha.-keto methylene group by reaction of the corresponding semicarbazones with SOCl2 or SeO2. The reactivity of I was also studied viz., Beckmann rearrangement, Shapiro reaction, Strecker synthesis of .alpha.-amino acids, etc.

IT **264129-41-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of annelated selenadiazoles and thiadiazoles from hydrothiapyranones.)

RN 264129-41-1 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-2,7-diphenyl-, (2R,7R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 7 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:98918 CAPLUS
DOCUMENT NUMBER: 132:148734
TITLE: Method and device for high-throughput screening of molecules and compounds for their effects on biological and chemical processes
INVENTOR(S): Stockwell, Brent R.; Schreiber, Stuart L.; Haggarty, Stephen J.; Mitchison, Timothy J.; Kapoor, Tarun M.; Mayer, Thomas
PATENT ASSIGNEE(S): President and Fellows of Harvard College, USA
SOURCE: PCT Int. Appl., 153 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000007017	A2	20000210	WO 1999-US17046	19990727
WO 2000007017	A3	20000504		
W: AU, CA, JP				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9953223	A1	20000221	AU 1999-53223	19990727

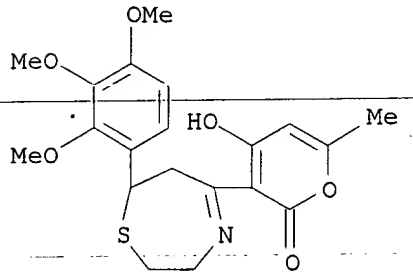
PRIORITY APPLN. INFO.:
US 1998-94305P P 19980727
US 1999-131765P P 19990430
US 1999-137039P P 19990601
WO 1999-US17046 W 19990727

OTHER SOURCE(S): MARPAT 132:148734

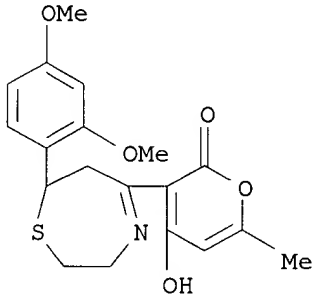
AB The present invention provides a system for high-throughput anal. of chem. compds. Assays are performed in a high d. platform, and compds. having pre-detd. desirable effects are identified. Preferably, the compds. have biol. effects, more preferably, the assays and detection are performed on whole cells. The system has a high-d. array of at least 100 reaction vessels, each vessel having a small vol. A 384-well 5-bromodeoxyuridine cytoblot assay was used to detect changes in DNA synthesis in mink lung cells caused by various agents.

IT **257292-28-7 257292-29-8 257292-30-1**
257292-31-2 257292-32-3 257292-33-4
257292-34-5 257292-35-6 257292-36-7
257292-37-8 257292-38-9 257292-39-0
257292-40-3 257292-41-4 257292-42-5
257292-43-6 257292-44-7
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(microtubules destabilization by; method and device for high-throughput screening of mols. and compds. for their effects on biol. and chem. processes)

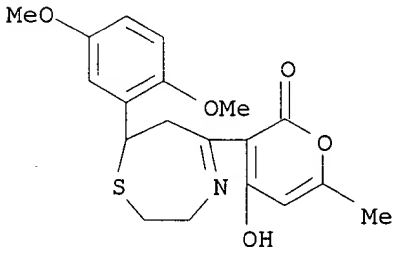
RN 257292-28-7 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2,3,4-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



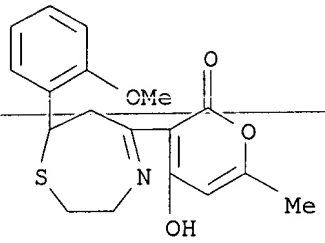
RN 257292-29-8 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,4-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



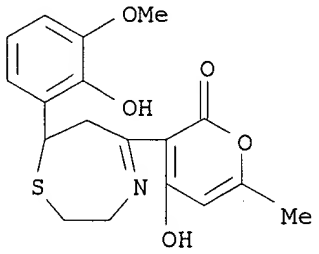
RN 257292-30-1 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,5-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



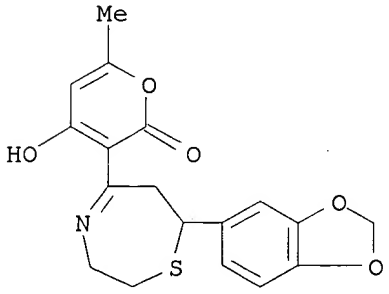
RN 257292-31-2 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



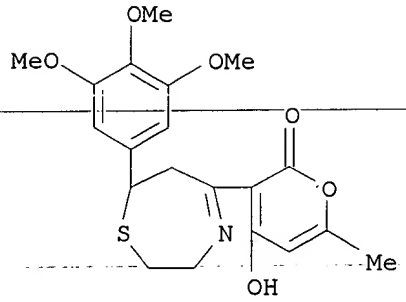
RN 257292-32-3 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2-hydroxy-3-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



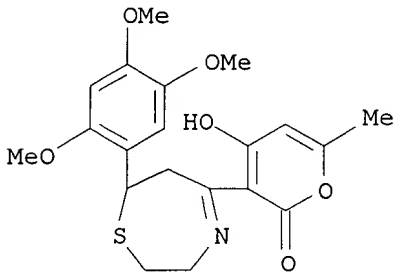
RN 257292-33-4 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(1,3-benzodioxol-5-yl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



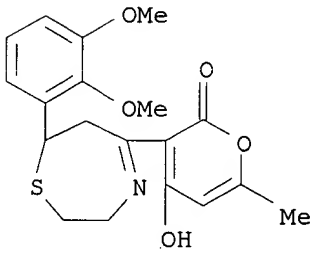
RN 257292-34-5 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(3,4,5-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



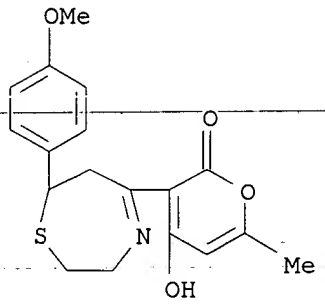
RN 257292-35-6 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(2,4,5-trimethoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



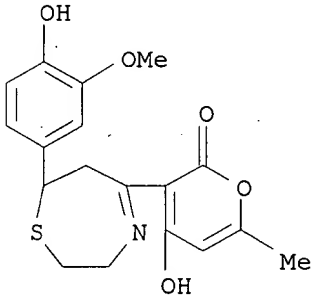
RN 257292-36-7 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(2,3-dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



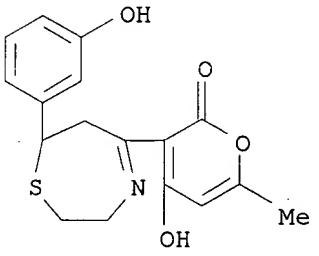
RN 257292-37-8 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(4-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



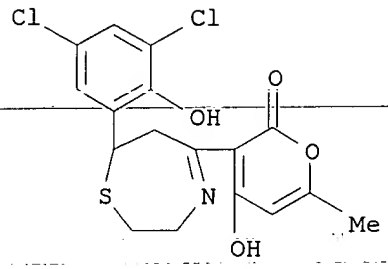
RN 257292-38-9 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(4-hydroxy-3-methoxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



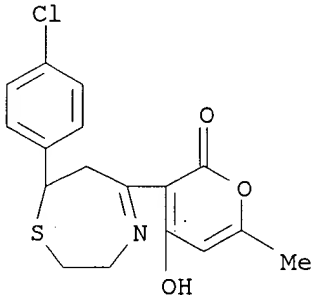
RN 257292-39-0 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(3-hydroxyphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



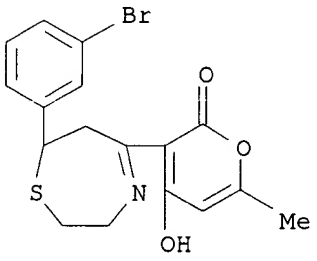
RN 257292-40-3 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(3,5-dichloro-2-hydroxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



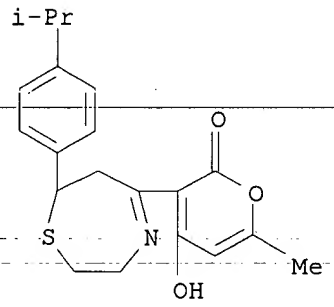
RN 257292-41-4 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(4-chlorophenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



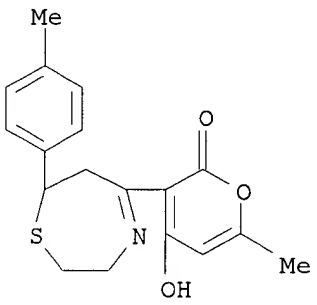
RN 257292-42-5 CAPLUS
CN 2H-Pyran-2-one, 3-[7-(3-bromophenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl- (9CI) (CA INDEX NAME)



RN 257292-43-6 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-[4-(1-methylethyl)phenyl]-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



RN 257292-44-7 CAPLUS
CN 2H-Pyran-2-one, 4-hydroxy-6-methyl-3-[2,3,6,7-tetrahydro-7-(4-methylphenyl)-1,4-thiazepin-5-yl]- (9CI) (CA INDEX NAME)



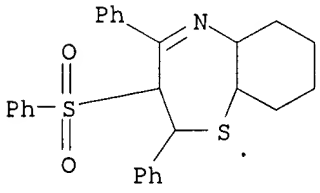
L13 ANSWER 8 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1994:245026 CAPLUS
DOCUMENT NUMBER: 120:245026
TITLE: Synthesis of 2,4-diaryl-3-(arylsulfonyl)-2,3-dihydro-1,5-benzothiazepines
AUTHOR(S): Reddey, D. Bhaskar; Sankaraiah, B.; Reddy, S.; Reddy, N. Subba; Reddy, P. V. Ramana
CORPORATE SOURCE: Dep. Chem., Sri Venkateswara Univ., Tirupati, 517 502, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1993), 32B(11), 1165-7
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

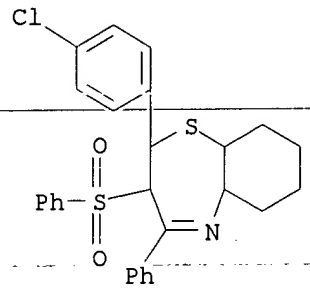
AB The reaction of 2-aminothiophenol with 1,3-diaryl-2-(arylsulfonyl)-2-propen-1-ones I (R1 = H, R2 = H, 4-Cl, 4-Br; R1 = 4-Cl, R2 = 4-Br; R1 = 4-Me, 4-Cl, R2 = H) in dry toluene at reflux temp. affords a mixt. of 1,3-diaryl-2-(arylsulfonyl)-3-(2'-aminophenylmercapto)-1-ones II and 2,4-diaryl-3-(arylsulfonyl)-2,3-dihydro-1,5-benzothiazepines III. The dehydrative cyclization of II yields III. The structures of II and III have been established by spectral data.

IT **154324-21-7P 154324-22-8P 154324-23-9P**
154324-24-0P 154324-25-1P 154324-26-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

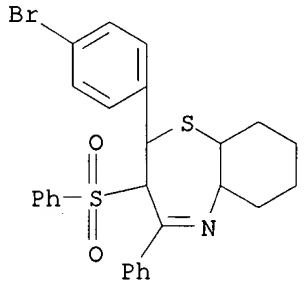
RN 154324-21-7 CAPLUS
CN 1,5-Benzothiazepine, 2,3,5a,6,7,8,9,9a-octahydro-2,4-diphenyl-3-(phenylsulfonyl)- (9CI) (CA INDEX NAME)



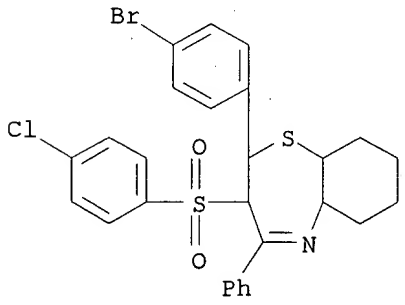
RN 154324-22-8 CAPLUS
CN 1,5-Benzothiazepine, 2-(4-chlorophenyl)-2,3,5a,6,7,8,9,9a-octahydro-4-phenyl-3-(phenylsulfonyl)- (9CI) (CA INDEX NAME)



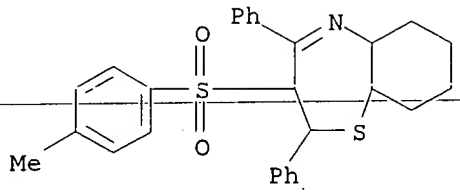
RN 154324-23-9 CAPLUS
CN 1,5-Benzothiazepine, 2-(4-bromophenyl)-2,3,5a,6,7,8,9,9a-octahydro-4-phenyl-3-(phenylsulfonyl)- (9CI) (CA INDEX NAME)



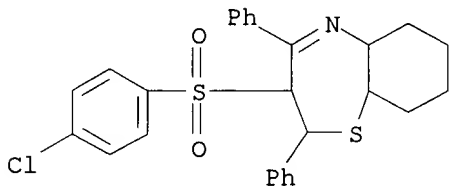
RN 154324-24-0 CAPLUS
CN 1,5-Benzothiazepine, 2-(4-bromophenyl)-3-[(4-chlorophenyl)sulfonyl]-2,3,5a,6,7,8,9,9a-octahydro-4-phenyl- (9CI) (CA INDEX NAME)



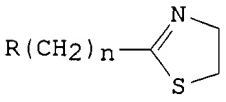
RN 154324-25-1 CAPLUS
CN 1,5-Benzothiazepine, 2,3,5a,6,7,8,9,9a-octahydro-3-[(4-methylphenyl)sulfonyl]-2,4-diphenyl- (9CI) (CA INDEX NAME)

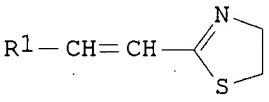


RN 154324-26-2 CAPLUS
CN 1,5-Benzothiazepine, 3-[(4-chlorophenyl)sulfonyl]-2,3,5a,6,7,8,9,9a-octahydro-2,4-diphenyl- (9CI) (CA INDEX NAME)



L13 ANSWER 9 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1993:539162 CAPLUS
DOCUMENT NUMBER: 119:139162
TITLE: Synthesis, antiparasitic and antifungal activities of arylalkyl and arylvinylthiazolines
AUTHOR(S): Caujolle, R.; Baziard-Mouysset, G.; Favrot, J. D.; Payard, M.; Loiseau, P. R.; Amarouch, H.; Linas, M. D.; Seguela, J. P.; Loiseau, P. M.; et al.
CORPORATE SOURCE: Dep. Chim., Fac. Pharm., Toulouse, 31000, Fr.
SOURCE: European Journal of Medicinal Chemistry (1993), 28(1), 29-35
CODEN: EJMCA5; ISSN: 0223-5234
DOCUMENT TYPE: Journal
LANGUAGE: French
GI

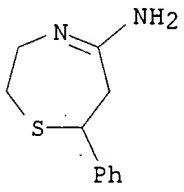

I


II

AB Twenty-seven arylalkyl- [I; R = Ph, n = 1, 2; R = 4-MeC6H4, 4-MeOC6H4, 3,4-(MeO)2C6H3, 4-ClC6H4, 4-O2NC6H4, 2-thienyl, 1-, 2-naphthyl, n = 1] or arylvinylthiazolines [II; R1 = Ph, 4-MeC6H4, 4-MeOC6H4, 4-MeSC6H4, 3,4-(MeO)2C6H3, 3,4-(OCH2O)C6H3, 4-ClC6H4, 2,4-Cl2C6H3, 4-O2NC6H4, 2-thienyl, 2-furyl, 2-, 3-, 4-pyridyl, 2-naphthyl, 2-benzofuryl, 2-(4-benzopyronyl)] were synthesized and tested in vitro against three genera of nematodes, various yeasts and opportunistic fungi. Vinyl compds. II seem to have an interesting filaricidal activity against Molinema dessetae and antifungal activity against yeasts.

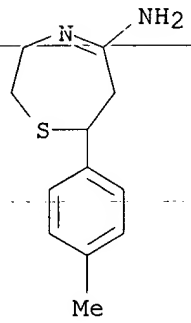
IT **149770-59-2P 149770-60-5P 149770-61-6P**
149770-62-7P 149770-63-8P 149770-64-9P
149770-65-0P 149770-66-1P 149770-67-2P
149770-68-3P 149770-69-4P 149770-70-7P
149770-71-8P 149770-72-9P 149770-73-0P
149770-74-1P 149770-75-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 149770-59-2 CAPLUS
CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-phenyl- (9CI) (CA INDEX NAME)

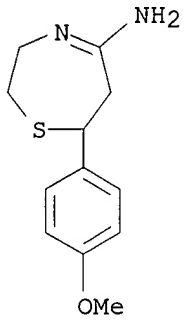


RN 149770-60-5 CAPLUS
CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-(4-methylphenyl)- (9CI) (CA

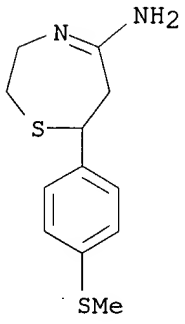
INDEX NAME)



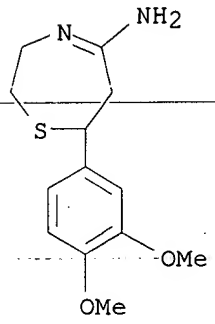
RN 149770-61-6 CAPLUS
CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



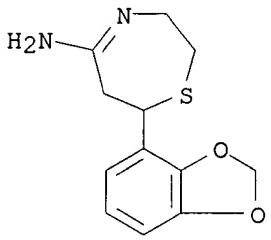
RN 149770-62-7 CAPLUS
CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-[4-(methylthio)phenyl]- (9CI) (CA INDEX NAME)



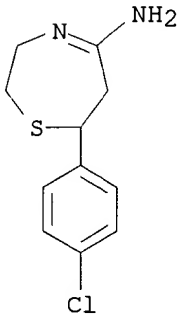
RN 149770-63-8 CAPLUS
CN 1,4-Thiazepin-5-amine, 7-(3,4-dimethoxyphenyl)-2,3,6,7-tetrahydro- (9CI) (CA INDEX NAME)



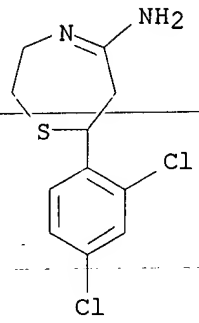
RN 149770-64-9 CAPLUS
CN 1,4-Thiazepin-5-amine, 7-(1,3-benzodioxol-4-yl)-2,3,6,7-tetrahydro- (9CI) (CA INDEX NAME)



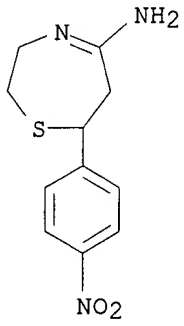
RN 149770-65-0 CAPLUS
CN 1,4-Thiazepin-5-amine, 7-(4-chlorophenyl)-2,3,6,7-tetrahydro- (9CI) (CA INDEX NAME)



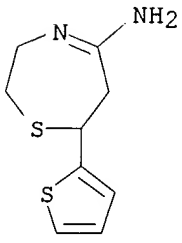
RN 149770-66-1 CAPLUS
CN 1,4-Thiazepin-5-amine, 7-(2,4-dichlorophenyl)-2,3,6,7-tetrahydro- (9CI) (CA INDEX NAME)



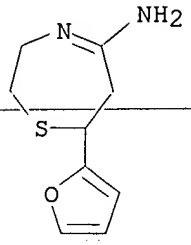
RN 149770-67-2 CAPLUS
CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



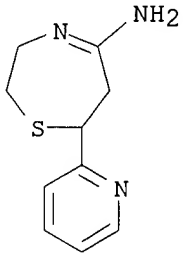
RN 149770-68-3 CAPLUS
CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-(2-thienyl)- (9CI) (CA INDEX NAME)



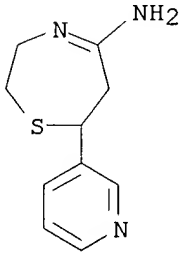
RN 149770-69-4 CAPLUS
CN 1,4-Thiazepin-5-amine, 7-(2-furanyl)-2,3,6,7-tetrahydro- (9CI) (CA INDEX NAME)



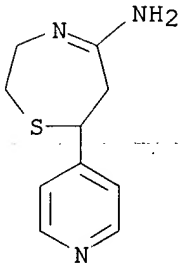
RN 149770-70-7 CAPLUS
CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-(2-pyridinyl)- (9CI) (CA INDEX NAME)



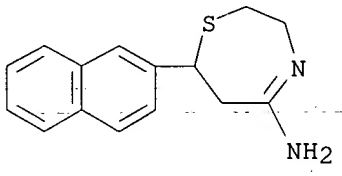
RN 149770-71-8 CAPLUS
CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-(3-pyridinyl)- (9CI) (CA INDEX NAME)



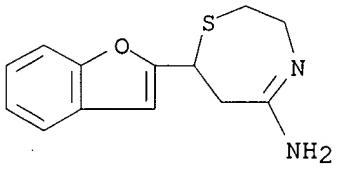
RN 149770-72-9 CAPLUS
CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-(4-pyridinyl)- (9CI) (CA INDEX NAME)



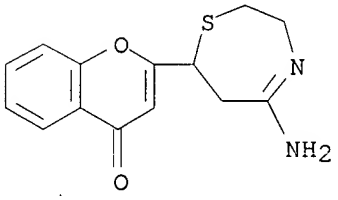
RN 149770-73-0 CAPLUS
CN 1,4-Thiazepin-5-amine, 2,3,6,7-tetrahydro-7-(2-naphthalenyl)- (9CI) (CA INDEX NAME)



RN 149770-74-1 CAPLUS
CN 1,4-Thiazepin-5-amine, 7-(2-benzofuranyl)-2,3,6,7-tetrahydro- (9CI) (CA INDEX NAME)



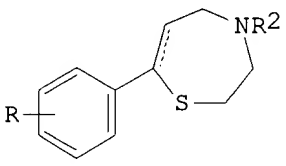
RN 149770-75-2 CAPLUS
CN 4H-1-Benzopyran-4-one, 2-(5-amino-2,3,6,7-tetrahydro-1,4-thiazepin-7-yl)- (9CI) (CA INDEX NAME)



L18 ANSWER 10 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1993:449417 CAPLUS
DOCUMENT NUMBER: 119:49417
TITLE: Preparation of substituted thiazepines as central nervous system agents
INVENTOR(S): Smith, William John; Wise, Lawrence David; Wustrow, David Juergen
PATENT ASSIGNEE(S): Warner-Lambert Co., USA
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9304053	A1	19930304	WO 1992-US6415	19920803
W: AU, CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE				
US 5206233	A	19930427	US 1991-750667	19910827
AU 9224370	A1	19930316	AU 1992-24370	19920803

PRIORITY APPLN. INFO.: US 1991-750667 19910827
WO 1992-US6415 19920803
OTHER SOURCE(S): MARPAT 119:49417
GI

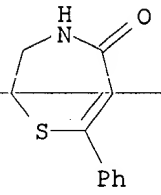


I

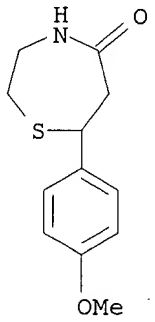
AB Title compds. I [R = H, alkyl, alkoxy, HO, halo, H2N, O2N, F3C, NC; R2 = H, alkyl, R3(CH2)n, R3(CH2)n, R3CO(CH2)n-1 wherein R3 = pyridyl, cycloalkyl, n = 1-5], isomers and a salt thereof, are prepd. I showed antipsychotic activity. H2MCH2CH2SH.cntdot.HCl, MeOH, NaOH and Me trans-4-metyoxycinnamate were reacted to give tetrahydro-7-(4-methoxyphenyl)-1,4-thiazepin-5-one which was treated with LiAlH4 and AlCl3 to give hexahydro-7-(4-methoxyphenyl)-1,4-thiazepine converted to HCl salt. Addnl. I were prepd.

IT **65922-92-1P 73920-60-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, in prepn. of central nervous system agents)

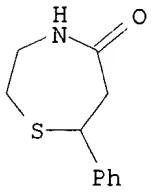
RN 65922-92-1 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, 3,4-dihydro-7-phenyl- (9CI) (CA INDEX NAME)



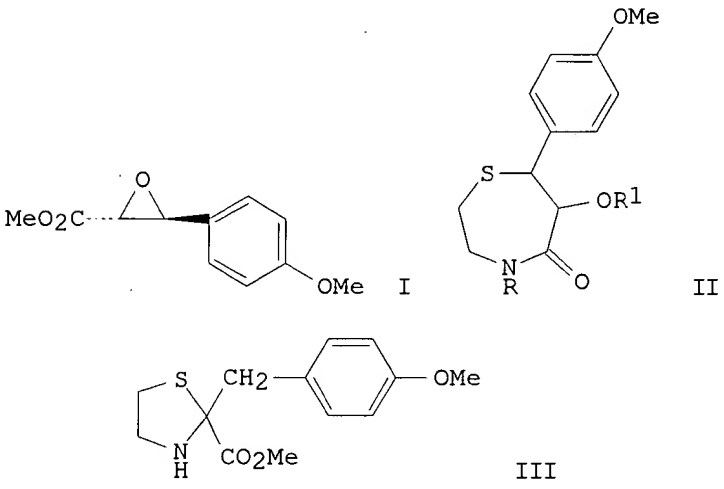
RN 73920-60-2 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



IT **2897-03-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, prepn. of thiazepine central nervous system agents)
RN 2897-03-2 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-phenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



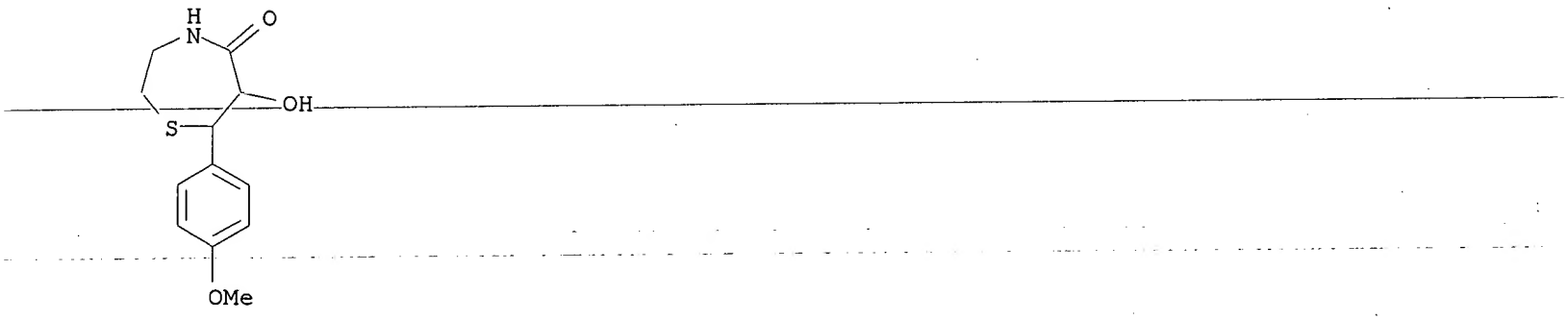
L13 ANSWER 11 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1992:426532 CAPLUS
DOCUMENT NUMBER: 117:26532
TITLE: Synthesis, stereochemistry and pharmacological activity of rac-cis-tetrahydro-6-hydroxy-7-(4-methoxyphenyl)-1,4-thiazepin-5(2H)-ones
AUTHOR(S): Mohacsi, Erno; O'Brien, Jay P.; Todaro, Louis J.
CORPORATE SOURCE: Roche Res. Cent., Hoffmann-La Roche Inc., Nutley, NJ, 07110, USA
SOURCE: Journal of Heterocyclic Chemistry (1992), 29(1), 193-7
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Reaction of 2-aminoethanethiol with trans-3-(p-methoxyphenyl)glycidate (I) gave the (.+-.)-cis-1,4-thiazepinone II (R = R1 = H) and a byproduct III. The structure of II (R = R1 = H) was proven by x-ray crystallog. The x-ray data revealed that this compd. adopts the chair conformation in the solid state and the heterocyclic ring is seven-membered. The structure of the byproduct III was elucidated on the basis of spectral data. II (R = CH2CH2NMe2, R1 = H, Ac) were inactive as calcium channel blocking agents.

IT **142011-35-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., alkylation with (dimethylamino)ethyl chloride and crystal and mol. structure of)

RN 142011-35-6 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-6-hydroxy-7-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)


H
N
O
OH
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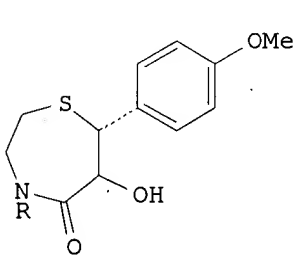
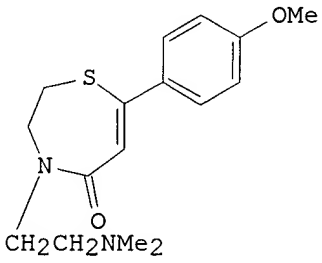
OMe

L13 ANSWER 12 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1992:106251 CAPLUS
DOCUMENT NUMBER: 116:106251
TITLE: The base-promoted dehydration of racemic trans-tetrahydro-6-hydroxy-4-[(2-(dimethylamino)ethyl]-7-(4-methoxyphenyl)-1,4-thiazepin-5(2H)-one
AUTHOR(S): Mohacsi, Erno; O'Brien, Jay P.
CORPORATE SOURCE: Roche Res. Cent., Hoffmann-La Roche Inc., Nutley, NJ, 07110, USA
SOURCE: Journal of Heterocyclic Chemistry (1991), 28(8), 2051-2
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

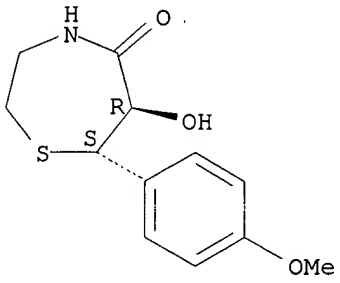
AB The base-catalyzed alkylation of racemic-trans-hydroxy(methoxyphenyl)thiazepinone I (R = H) with dimethylaminoethyl chloride in DMSO provided predominantly I (R = CH2CH2NMe2) and also dihydro[(dimethylamino)ethyl](methoxyphenyl)thiazepinone II.

IT **130056-74-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation of, with (dimethylamino)ethyl chloride)

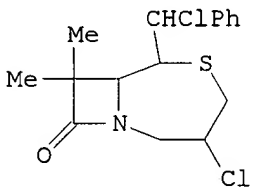
RN 130056-74-5 CAPLUS

CN 1,4-Thiazepin-5(2H)-one, tetrahydro-6-hydroxy-7-(4-methoxyphenyl)-, trans- (9CI) (CA INDEX NAME)

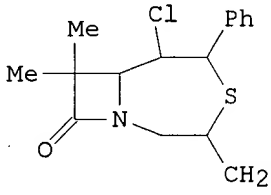
Relative stereochemistry.



L13 ANSWER 13 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1991:491900 CAPLUS
DOCUMENT NUMBER: 115:91900
TITLE: Novel synthesis of thianonanam using sulfur dichloride as a sulfur transfer reagent
AUTHOR(S): Komatsu, Mitsuo; Mohri, Masaaki; Kume, Shoichiro; Ohshiro, Yoshiki
CORPORATE SOURCE: Fac. Eng., Osaka Univ., Suita, 565, Japan
SOURCE: Heterocycles (1991), 32(4), 659-62
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:91900
GI



I



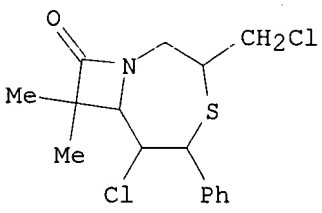
II

AB Thianonanams I and II were synthesized by addn. of SCl2 to N-allyl-.beta.-styryl-.beta.-lactam.

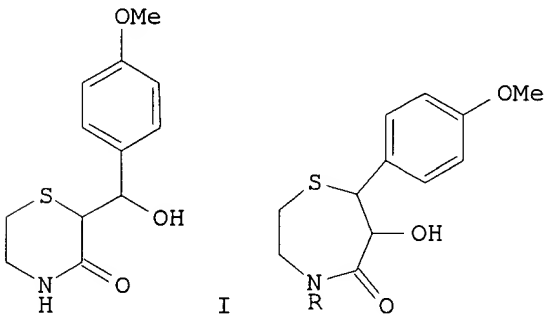
IT **135299-43-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 135299-43-3 CAPLUS

CN 4-Thia-1-azabicyclo[5.2.0]nonan-9-one, 6-chloro-3-(chloromethyl)-8,8-dimethyl-5-phenyl- (9CI) (CA INDEX NAME)



L13 ANSWER 14 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1990:591311 CAPLUS
DOCUMENT NUMBER: 113:191311
TITLE: Synthesis and stereochemistry of rac.-trans-tetrahydro-6-hydroxy-7-(4-methoxyphenyl)-1,4-thiazepin-5(2H)-one
AUTHOR(S): Mohacsi, Erno; O'Brien, Jay P.; Todaro, Louis J.
CORPORATE SOURCE: Chem. Res. Dep., Hoffmann-La Roche Inc., Nutley, NJ, 07110, USA
SOURCE: Journal of Heterocyclic Chemistry (1990), 27(4), 1085-89
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:191311
GI



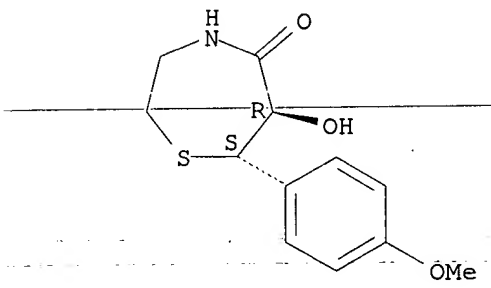
AB The base catalyzed reaction of NH2CH2CH2SH with Me trans-3-(p-methoxyphenyl)glycidate gave a mixt. of isomeric lactams I and II (R = H) and in addn., a byproduct 4H-2,3,5,6-tetrahydro[1,3]thiazin-3-one. The structures of I and II (R = CH2CH2NMe2) were detd. by x-ray crystallog. The data revealed that both isomers adopt the chair conformation in the solid state.

IT **130056-74-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

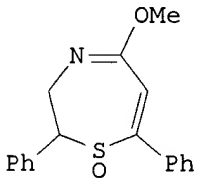
RN 130056-74-5 CAPLUS

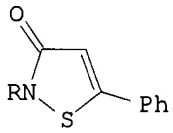
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-6-hydroxy-7-(4-methoxyphenyl)-, trans-(9CI) (CA INDEX NAME)

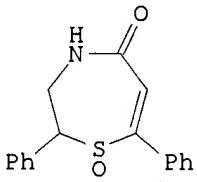
Relative stereochemistry.


H
N
O
R
OH
S
S
OMe

L3 ANSWER 15 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1987:617608 CAPLUS
DOCUMENT NUMBER: 107:217608
TITLE: Ring-contraction reactions of dihydro- and tetrahydrothiazepines to isothiazolone derivatives under Pummerer conditions
AUTHOR(S): Yamamoto, Kagetoshi; Yamazaki, Shoko; Murata, Ichiro; Fukazawa, Yoshimasa
CORPORATE SOURCE: Fac. Sci., Osaka Univ., Toyonaka, 560, Japan
SOURCE: Journal of Organic Chemistry (1987), 52(23), 5239-43
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 107:217608
GI


I

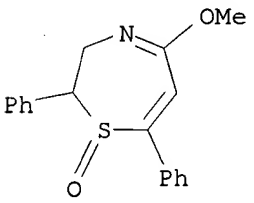

II


III

AB Thiazepine oxide I underwent Pummerer reaction (NaOAc in Ac2O) to give styrylisothiazole II (R = cis-PhCH:CH) which isomerized to the trans-isomer upon heating. Similarly, sulfoxide III underwent ring contraction to give II (R = trans-PhCH:CH) and 2-acetoxy-4,5-diphenylpyridine. However, upon treatment with (CF3CO)2O, III gave oxoisothiazole II [R = PhCH(O2CCF3)CH2]. A mechanism for these ring contractions, which involves a common bicyclic intermediate, is suggested.

IT **110567-89-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and Pummerer reaction of, phenylstyrylisothiazole from)

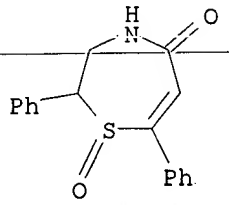
RN 110567-89-0 CAPLUS
CN 1,4-Thiazepine, 2,3-dihydro-5-methoxy-2,7-diphenyl-, 1-oxide (9CI) (CA INDEX NAME)



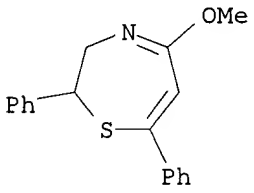
IT **110567-92-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and Pummerer reaction of, with acetic anhydride or trifluoroacetic anhydride)

RN 110567-92-5 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, 3,4-dihydro-2,7-diphenyl-, 1-oxide (9CI) (CA

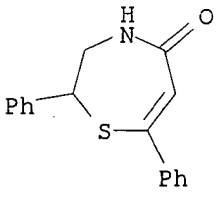
INDEX NAME)



IT **110567-88-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and chloroperbenzoic acid oxidn. of)
RN 110567-88-9 CAPLUS
CN 1,4-Thiazepine, 2,3-dihydro-5-methoxy-2,7-diphenyl- (9CI) (CA INDEX NAME)



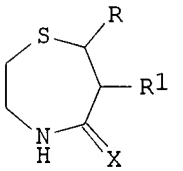
IT **110567-87-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., chloroperbenzoic acid oxidn., or O-methylation of, with trimethyloxonium tetrafluoroborate)
RN 110567-87-8 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, 3,4-dihydro-2,7-diphenyl- (9CI) (CA INDEX NAME)



L13 ANSWER 16 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1986:608947 CAPLUS
DOCUMENT NUMBER: 105:208947
TITLE: 1,4-Thiazepinethiones as plant fungicides
INVENTOR(S): Nishihata, Takeshi; Saito, Toshinori; Yasufuku, Kazue; Fukatsu, Shunzo; Matsumoto, Kuniomi; Watanabe, Tetsuo
PATENT ASSIGNEE(S): Meiji Seika Kaisha, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61083176	A2	19860426	JP 1984-206015	19841001

OTHER SOURCE(S): CASREACT 105:208947
GI

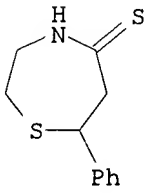


I

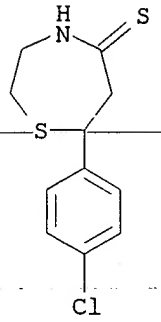
AB The title compds. [I; R, R1 = H, C1-5 alkyl, (substituted) aryl, aralkyl; X = S], useful as plant fungicides, were prepd., e.g., by treating I (X = O) with P2S5 or Lawesson's reagent. Thus, heating a suspension of 1.73 g I (R = CHMe2, R1 = H, X = O) in 70 mL pyridine with 2.31 g P2S5 at 90.degree. for 30 min gave 0.75 g I (R = CHMe2, R1 = H, X = S), which was as effective as Hinosan against rice blast.

IT **105150-99-0P 105151-01-7P 105151-02-8P**
105151-03-9P 105151-05-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as plant fungicide)

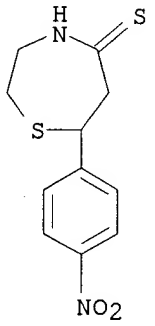
RN 105150-99-0 CAPLUS
CN 1,4-Thiazepine-5(2H)-thione, tetrahydro-7-phenyl- (9CI) (CA INDEX NAME)



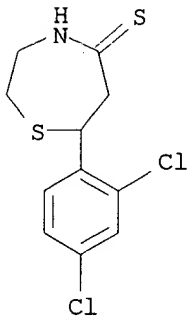
RN 105151-01-7 CAPLUS
CN 1,4-Thiazepine-5(2H)-thione, 7-(4-chlorophenyl)tetrahydro- (9CI) (CA INDEX NAME)



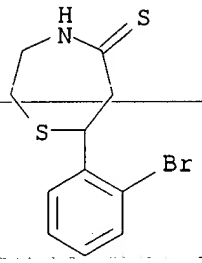
RN 105151-02-8 CAPLUS
CN 1,4-Thiazepine-5(2H)-thione, tetrahydro-7-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



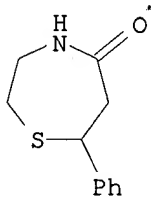
RN 105151-03-9 CAPLUS
CN 1,4-Thiazepine-5(2H)-thione, 7-(2,4-dichlorophenyl)tetrahydro- (9CI) (CA INDEX NAME)



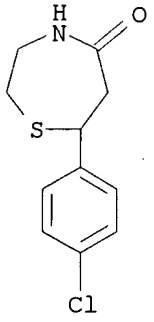
RN 105151-05-1 CAPLUS
CN 1,4-Thiazepine-5(2H)-thione, 7-(2-bromophenyl)tetrahydro- (9CI) (CA INDEX NAME)



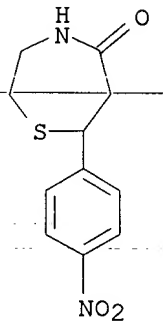
IT **2897-03-2 105151-08-4 105151-09-5**
105151-10-8 105151-12-0
RL: RCT (Reactant)
(sulfuration of, with phosphorus pentasulfide)
RN 2897-03-2 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-phenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



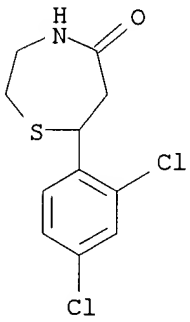
RN 105151-08-4 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, 7-(4-chlorophenyl)tetrahydro- (9CI) (CA INDEX NAME)



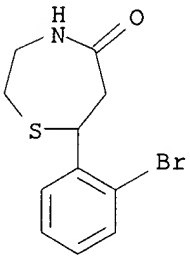
RN 105151-09-5 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



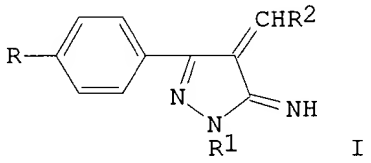
RN 105151-10-8 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, 7-(2,4-dichlorophenyl)tetrahydro- (9CI) (CA INDEX NAME)



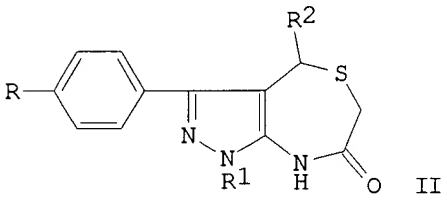
RN 105151-12-0 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, 7-(2-bromophenyl)tetrahydro- (9CI) (CA INDEX NAME)



L18 ANSWER 17 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1981:15694 CAPLUS
DOCUMENT NUMBER: 94:15694
TITLE: Investigation of the reaction products of 5-amino-1,3-disubstitutedpyrazoles with aromatic aldehydes. Synthesis of new fluorinated 1,3,4-trisubstituted-1H-pyrazolo[3,4-e][1,4]thiazepin-7-ones
AUTHOR(S): Joshi, Krishna C.; Pathak, Vijai N.; Garg, Urmila
CORPORATE SOURCE: Dep. Chem., Univ. Rajasthan, Jaipur, 302004, India
SOURCE: J. Heterocycl. Chem. (1980), 17(4), 789-91
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



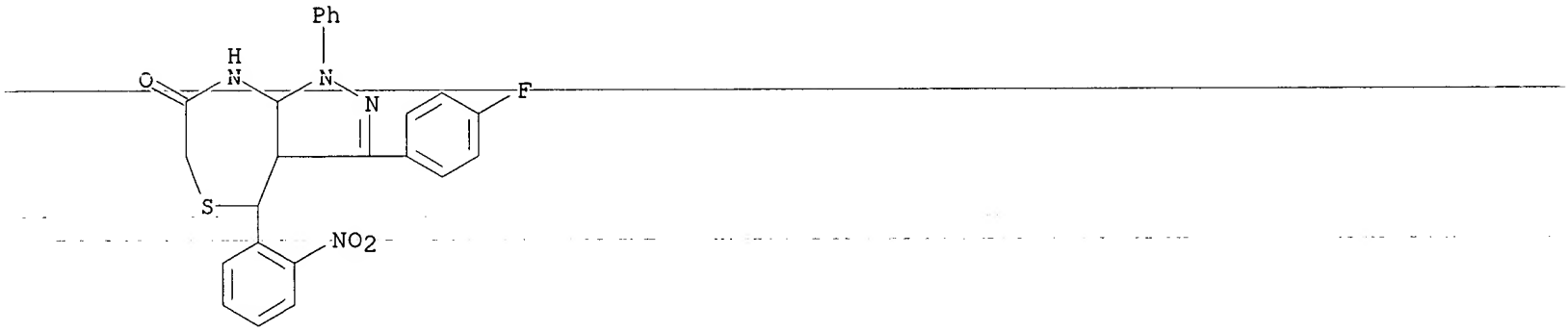
I



II

AB The condensation products of 1,3-disubstituted 5-aminopyrazoles with arom. aldehydes were identified as phenylmethylenepyrazolimine derivs. I (R = F, H, R1 = Ph, p-ClC6H4, p-FC6H4, C6F4, p-MeC6H4SO2, p-FC6H4SO2; R2 = substituted Ph). Treatment I with mercaptoacetic acid gave new fluorine contg. pyrazolothiazepinones II.

IT **76058-84-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and proton and fluorine-19 NMR of)
RN 76058-84-9 CAPLUS
CN 1H-Pyrazolo[3,4-e][1,4]thiazepin-7(6H)-one, 3-(4-fluorophenyl)-3a,4,8,8a-tetrahydro-4-(2-nitrophenyl)-1-phenyl- (9CI) (CA INDEX NAME)


Ph
H
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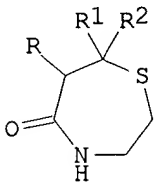
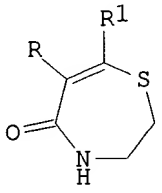
N
F
S
NO2

L13 ANSWER 18 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:408144 CAPLUS
DOCUMENT NUMBER: 93:8144
TITLE: Chlorination-dehydrochlorination of perhydro-1,4-thiazepin-5-ones
AUTHOR(S): Wamhoff, Heinrich; Theis, Christoph H.
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, D-5300/1, Fed. Rep. Ger.
SOURCE: Chem. Ber. (1980), 113(3), 995-1009
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
GI


I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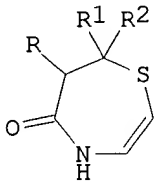
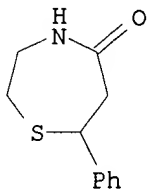
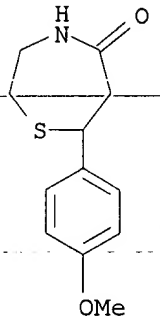

III

AB Chlorination of the thiazepinones I (R = R2 = H, R1 = H, Me, Ph, 4-MeOC6H4; R = Me, Ph, R1 = R2 = H; R = H, R1 = R2 = Me) with SO2Cl2 or N-chlorosuccinimide, followed by dehydrochlorination, gave II and III. Reaction with Me3COCl gave the S-oxides of I in addn. to the chlorination products. Halogenation of II (R = H, R1 = H, Me, Ph) with SO2Cl2 or Br gave II (R = Cl, Br).

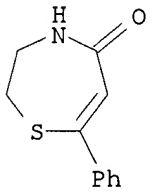
IT **2897-03-2**
RL: RCT (Reactant)
(chlorination-dehydrochlorination of)
RN 2897-03-2 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-phenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



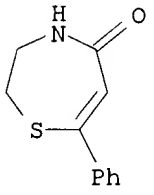
IT **73920-60-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and chlorination-dehydrochlorination of)
RN 73920-60-2 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



IT **65922-92-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and halogenation of)
RN 65922-92-1 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, 3,4-dihydro-7-phenyl- (9CI) (CA INDEX NAME)

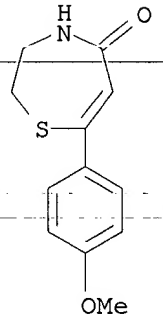


IT **73920-73-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and neutralization of)
RN 73920-73-7 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, 3,4-dihydro-7-phenyl-, hydrochloride (9CI) (CA INDEX NAME)

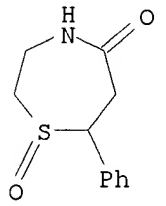


HCl

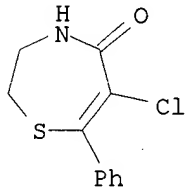
IT **73920-66-8P 73920-74-8P 73920-79-3P**
73920-81-7P 73920-82-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 73920-66-8 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, 3,4-dihydro-7-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



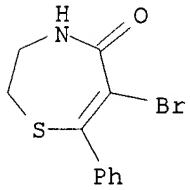
RN 73920-74-8 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-phenyl-, 1-oxide (9CI) (CA INDEX NAME)



RN 73920-79-3 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, 6-chloro-3,4-dihydro-7-phenyl- (9CI) (CA INDEX NAME)

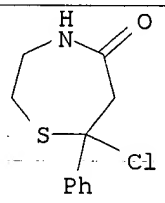


RN 73920-81-7 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, 6-bromo-3,4-dihydro-7-phenyl- (9CI) (CA INDEX NAME)

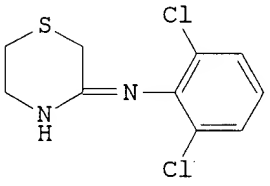


RN 73920-82-8 CAPLUS

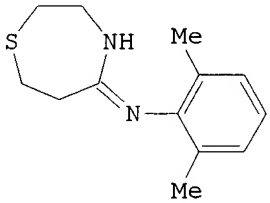
CN 1,4-Thiazepin-5(2H)-one, 7-chlorotetrahydro-7-phenyl- (9CI) (CA INDEX NAME)



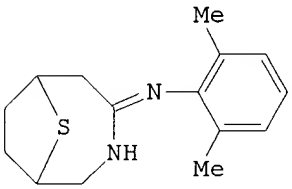
L3 ANSWER 19 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1978:152525 CAPLUS
DOCUMENT NUMBER: 88:152525
TITLE: Antihypertensive agents: Part V. Synthesis and antihypertensive activity of 3-arylimino-2,3,5,6-tetrahydro-4H-1,4-thiazines and related cyclic amidines
AUTHOR(S): Arya, V. P.; Kaul, C. L.; Grewal, R. S.; David, J.; Talwalker, P. K.; Shenoy, S. J.
CORPORATE SOURCE: Res. Cent., Ciba-Geigy, Bombay, India
SOURCE: Indian J. Chem., Sect. B (1977), 15(8), 720-6
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



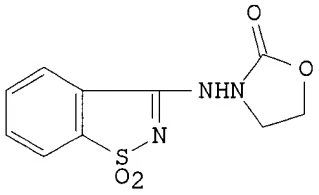
I



II



III



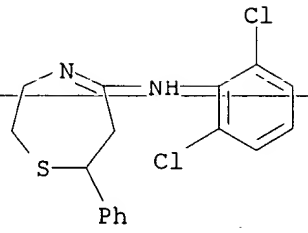
IV

AB 3-Arylimino-2,3,5,6-tetrahydro-4H-1,4-thiazines, e.g., I, were prepd. from thiamorpholin-3-one, POCl3, and anilines for antihypertensive screening. The corresponding 1,4-oxazines were prepd. from substituted morpholin-3-ones, POCl3, and substituted anilines. Seven- and eight-membered cyclic amidines, e.g., II, were prepd. by treating the corresponding lactams with POCl3 and substituted anilines. A novel heterocyclic amidine III, was prepared from tropinone; IV was also prepd. The structure-activity relationship of the cyclic amidines was reported.

IT **65922-96-5P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and antihypertensive activity of)

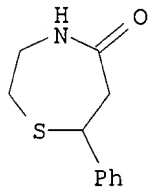
RN 65922-96-5 CAPLUS

CN 1,4-Thiazepin-5-amine, N-(2,6-dichlorophenyl)-2,3,6,7-tetrahydro-7-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

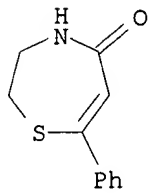


● HCl

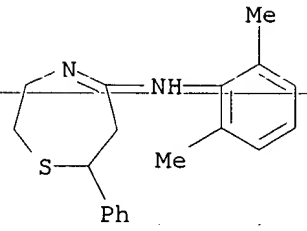
IT **2897-03-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with anilines)
RN 2897-03-2 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-phenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



IT **65922-92-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation with dimethylaniline)
RN 65922-92-1 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, 3,4-dihydro-7-phenyl- (9CI) (CA INDEX NAME)

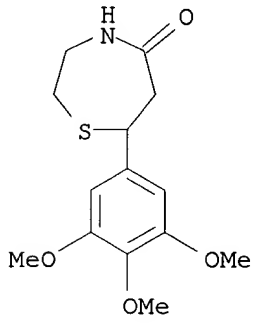


IT **65922-97-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and pharmacol. activity of)
RN 65922-97-6 CAPLUS
CN 1,4-Thiazepin-5-amine, N-(2,6-dimethylphenyl)-2,3,6,7-tetrahydro-7-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

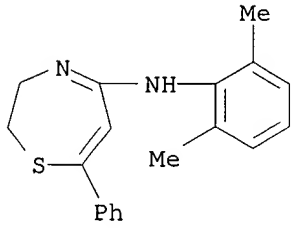


● HCl

IT **65922-91-0P 65923-18-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 65922-91-0 CAPLUS
CN 1,4-Thiazepin-5(2H)-one, tetrahydro-7-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

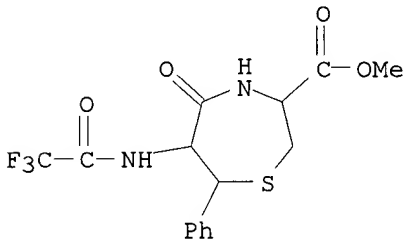


RN 65923-18-4 CAPLUS
CN 1,4-Thiazepin-5-amine, N-(2,6-dimethylphenyl)-2,3-dihydro-7-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L13 ANSWER 20 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1976:165182 CAPLUS
DOCUMENT NUMBER: 84:165182
TITLE: Synthesis of some dehydrophenylalanine peptides
AUTHOR(S): Breitholle, Edward G.; Stammer, Charles H.
CORPORATE SOURCE: Chem. Dep., Univ. Georgia, Athens, Ga., USA
SOURCE: J. Org. Chem. (1976), 41(8), 1344-9
CODEN: JOCEAH
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Addnl. data considered in abstracting and indexing are available from a source cited in the original document. The bromo pseudoazlactones, (I, R1 = H, Me, Ph, Me2CH, Et, R2 = H, Me), dehydrobrominated readily giving the unsatd. azlactones, II, which were converted into N-trifluoroacetyldehydro amino acid anilides and peptides and perhydro-1,4-thiazepin-5-ones. N-trifluoroacetyldehydrovaline, isoleucine, leucine, alanine, and aminobutyric acid anilides and peptides were not deblocked by NH3. Treatment of I (R1 = Ph, R2 = H) in DMF contg. Et3N with Phe-OMe gave 76% PhCH:C(NHCOCF3)CONHCH(CH2Ph)CO2Me.
IT **58219-84-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 58219-84-4 CAPLUS
CN 1,4-Thiazepine-3-carboxylic acid, hexahydro-5-oxo-7-phenyl-6-[(trifluoroacetyl)amino]-, methyl ester (9CI) (CA INDEX NAME)

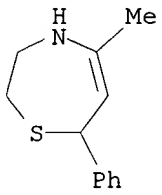


L13 ANSWER 21 OF 21 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1975:3907 CAPLUS
DOCUMENT NUMBER: 82:3907
TITLE: Reaction products from 4-phenylbut-3-yn-2-one and aliphatic diamines or 2-aminoethanethiol, and from 2-aminoethanethiol and .alpha.,.beta.-enones
AUTHOR(S): Hankovszky, Olga H.; Hideg, Kalman; Lloyd, Douglas
CORPORATE SOURCE: Cent. Lab. Chem., Univ. Pecs, Pecs, Hung.
SOURCE: J. Chem. Soc., Perkin Trans. 1 (1974), (14), 1619-21
CODEN: JCPRB4
DOCUMENT TYPE: Journal
LANGUAGE: English

AB PhC.tplbond.CCOMe with H2N(CH2)nNH2 (n = 2, 3) in the presence and absence of Na2CO3 gave MeCOCH:CPhNH(CH2)nNHCPh:CHCOMe and PhC.tplbond.CCMe:N(CH2)nN:CMeC.tplbond.CPh, resp. H2N(CH2)2SH with PhC.tplbond.CCOMe gave MeCOCH:CPhNH(CH2)2SH, with PhCH:CHCOMe gave 2,3,6,7- and/or 2,3,4,7-tetrahydro-5-methyl-7-phenyl-1,4-thiazepine, and with chalcone gave PhCOCH2CHPhNH(CH2)2SH and PhCOCH2CHPhS(CH2)2NH2 or PhCOCH2CHPhS(CH2)2NHCHPhCH2COPh depending on the molar ratios used.

IT **54454-44-3P 54454-45-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 54454-44-3 CAPLUS
CN 1,4-Thiazepine, 2,3,4,7-tetrahydro-5-methyl-7-phenyl- (9CI) (CA INDEX NAME)



RN 54454-45-4 CAPLUS
CN 1,4-Thiazepine, 2,3,6,7-tetrahydro-5-methyl-7-phenyl- (9CI) (CA INDEX NAME)